



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2017 – 08:35 PM EDT

PDB ID : 1QO5
Title : Fructose 1,6-bisphosphate Aldolase from Human Liver Tissue
Authors : Dalby, A.R.; Littlechild, J.A.
Deposited on : unknown
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

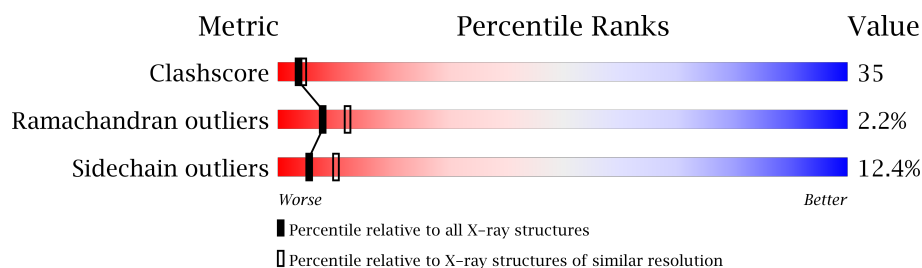
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	
1	G	363	

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Mol	Chain	Length	Quality of chain
1	H	363	
1	I	363	
1	J	363	
1	K	363	
1	L	363	
1	M	363	
1	N	363	
1	O	363	
1	P	363	
1	Q	363	
1	R	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	401	-	-	X	-
2	SO4	A	402	-	-	X	-
2	SO4	D	400	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called FRUCTOSE-BISPHOSPHATE ALDOLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2730	1708	486	521	15			
1	B	348	Total	C	N	O	S	0	0	0
			2651	1660	473	504	14			
1	C	345	Total	C	N	O	S	0	0	0
			2635	1652	470	499	14			
1	D	356	Total	C	N	O	S	0	0	0
			2701	1689	482	516	14			
1	E	354	Total	C	N	O	S	0	0	0
			2687	1680	480	513	14			
1	F	353	Total	C	N	O	S	0	0	0
			2675	1674	474	513	14			
1	G	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	H	357	Total	C	N	O	S	0	0	0
			2712	1698	483	517	14			
1	I	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	J	356	Total	C	N	O	S	0	0	0
			2701	1689	482	516	14			
1	K	354	Total	C	N	O	S	0	0	0
			2686	1683	475	514	14			
1	L	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	M	360	Total	C	N	O	S	29	0	0
			2730	1708	486	521	15			
1	N	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	O	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	P	360	Total	C	N	O	S	0	0	0
			2730	1708	486	521	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	R	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	34	Total	O	0	0
			34	34		
3	C	44	Total	O	0	0
			44	44		
3	D	82	Total	O	0	0
			82	82		
3	E	75	Total	O	0	0
			75	75		
3	F	80	Total	O	0	0
			80	80		
3	G	75	Total	O	0	0
			75	75		
3	H	70	Total	O	0	0
			70	70		
3	I	45	Total	O	0	0
			45	45		
3	J	78	Total	O	0	0
			78	78		
3	K	71	Total	O	0	0
			71	71		
3	L	28	Total	O	0	0
			28	28		
3	M	81	Total	O	0	0
			81	81		

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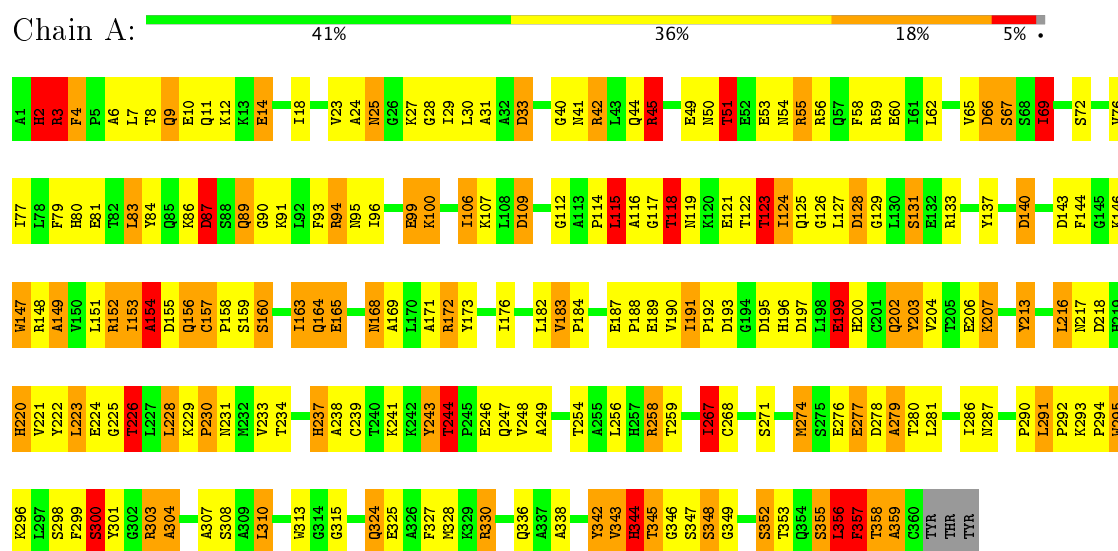
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	53	Total 53	O 53	0	0
3	O	37	Total 37	O 37	0	0
3	P	78	Total 78	O 78	0	0
3	Q	80	Total 80	O 80	0	0
3	R	72	Total 72	O 72	0	0

3 Residue-property plots

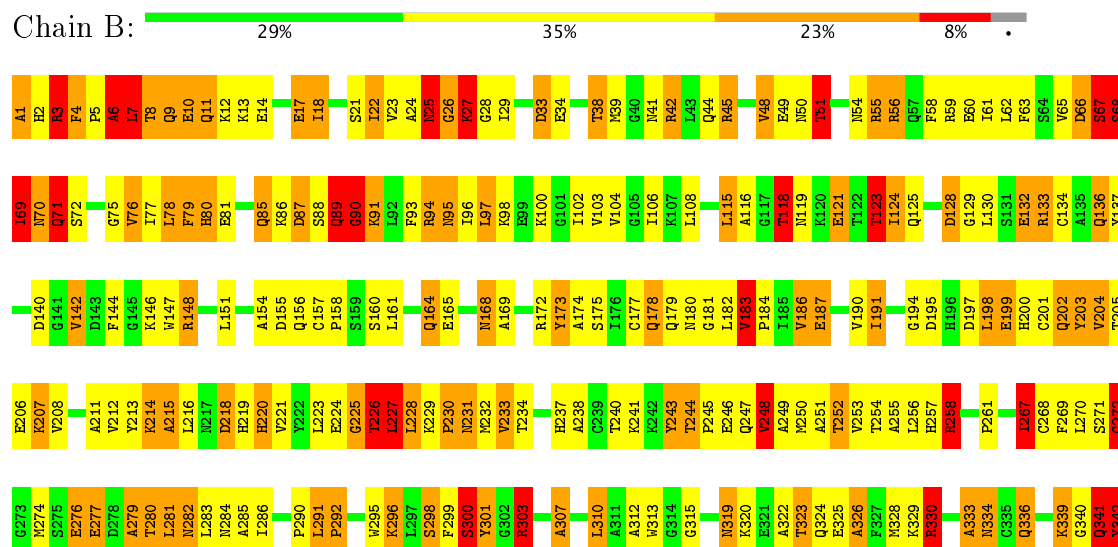
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

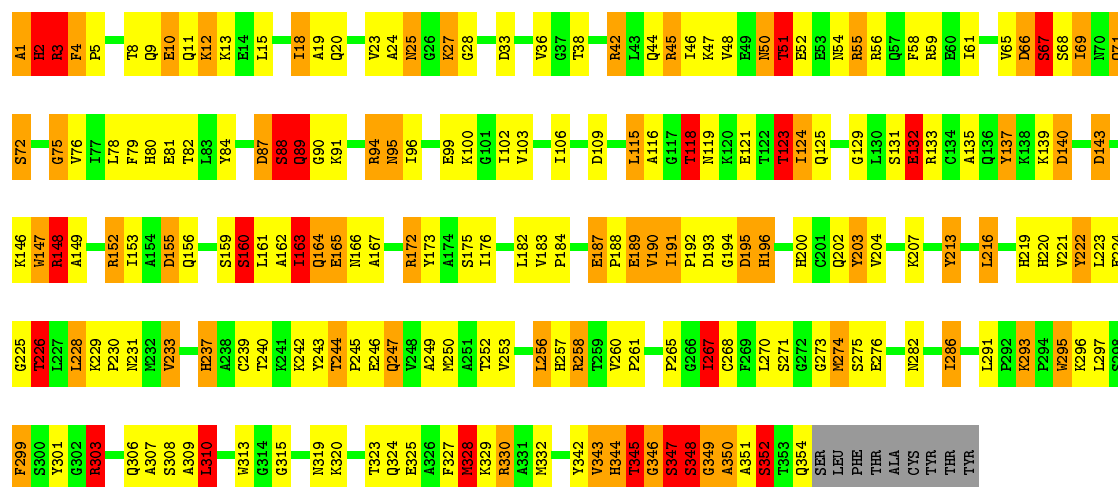
Note EDS was not executed.

• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

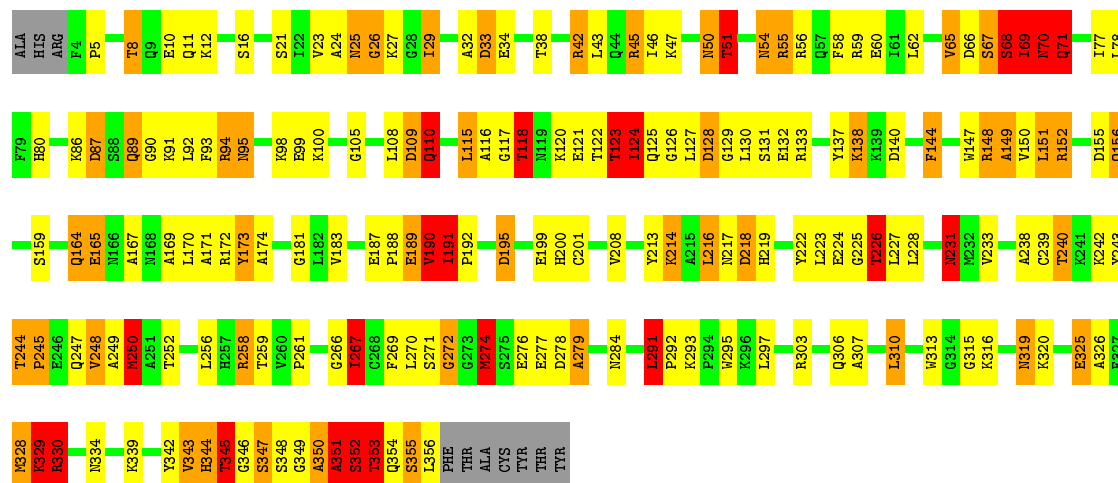


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

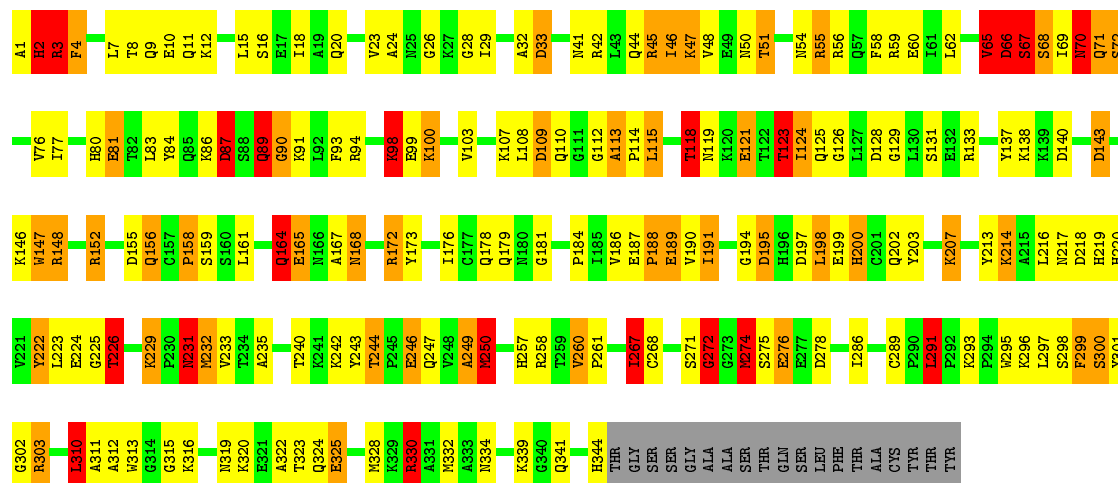




- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

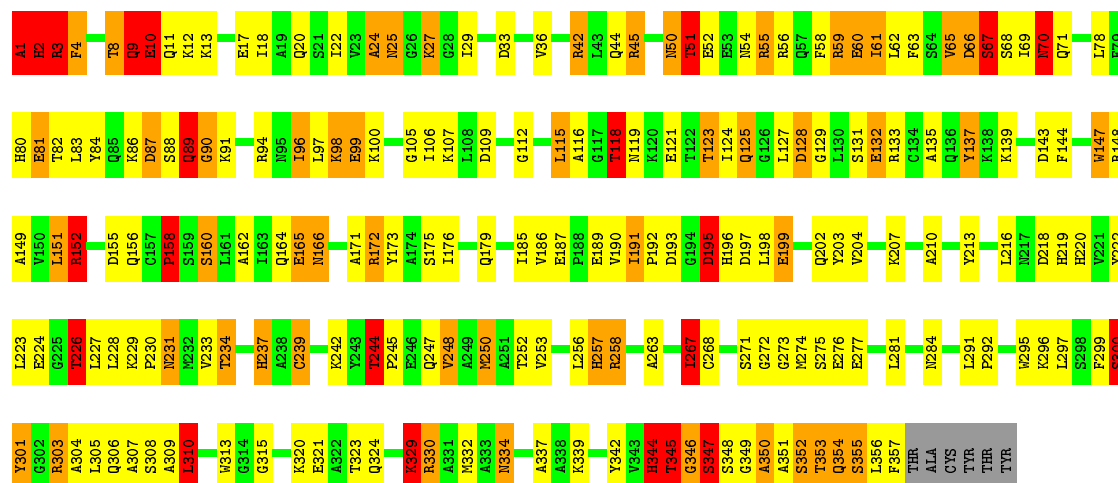


- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



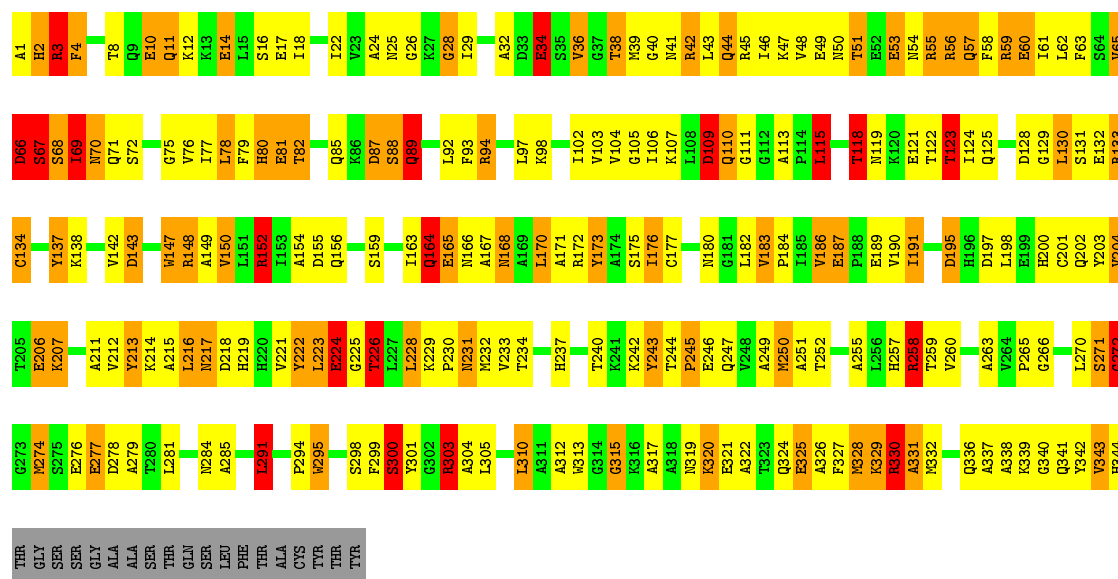
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain H:  42% 36% 14% 6%



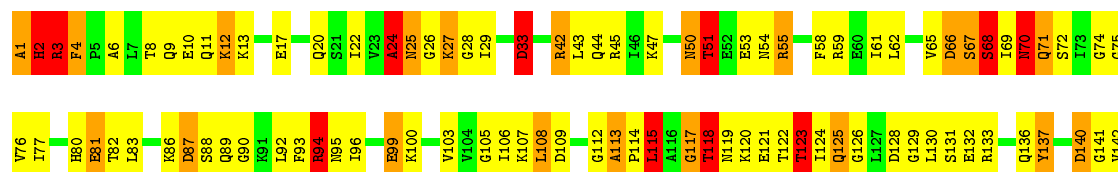
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

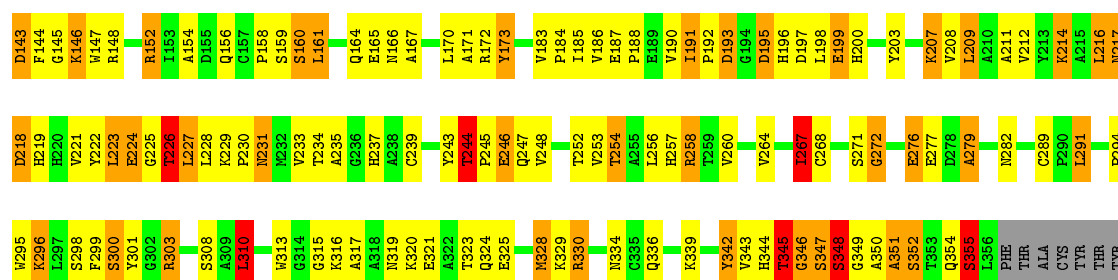
Chain I: 



- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

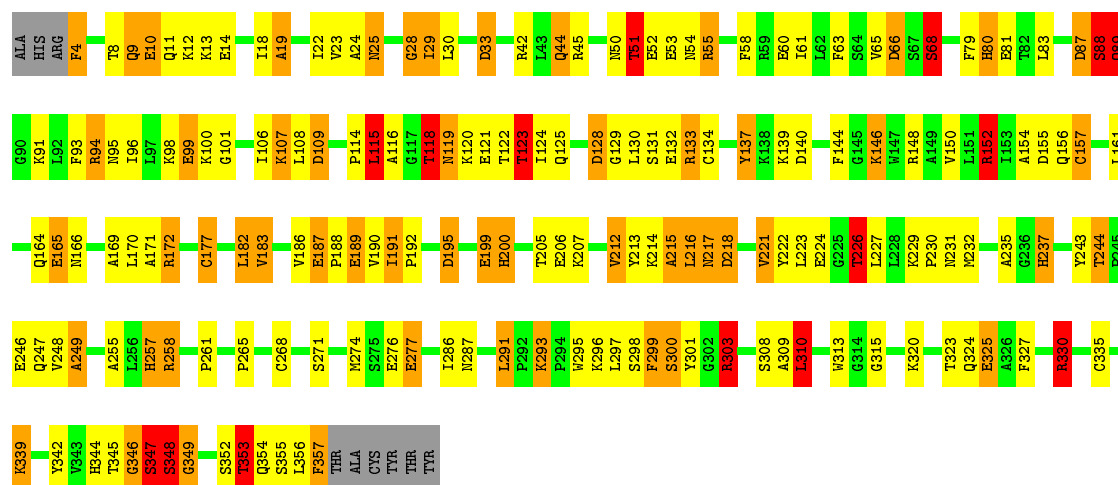
Chain J: 37% 40% 16% 5% .





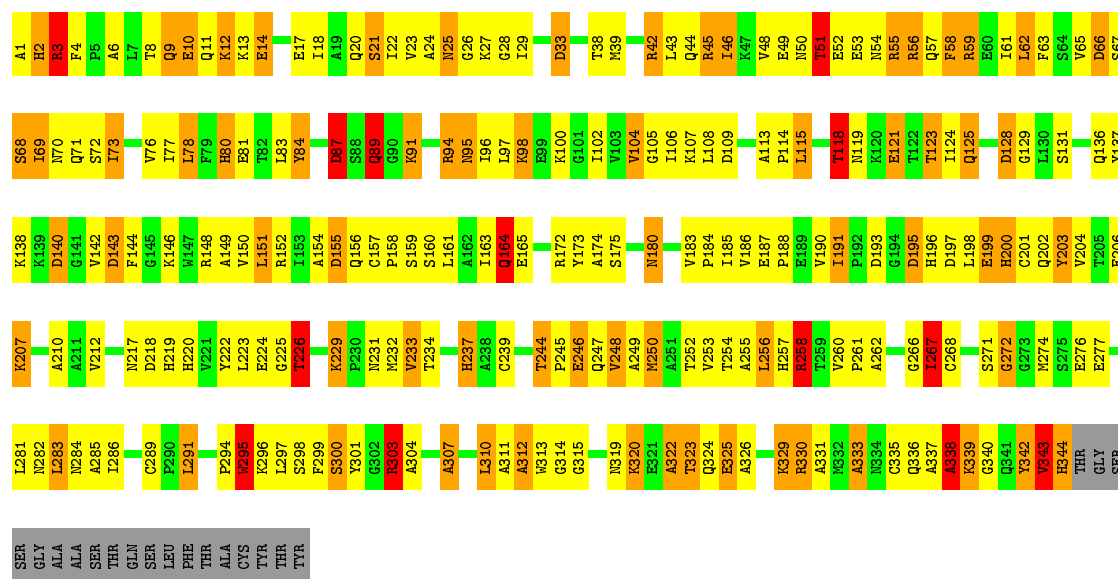
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain K: 48% 31% 15%

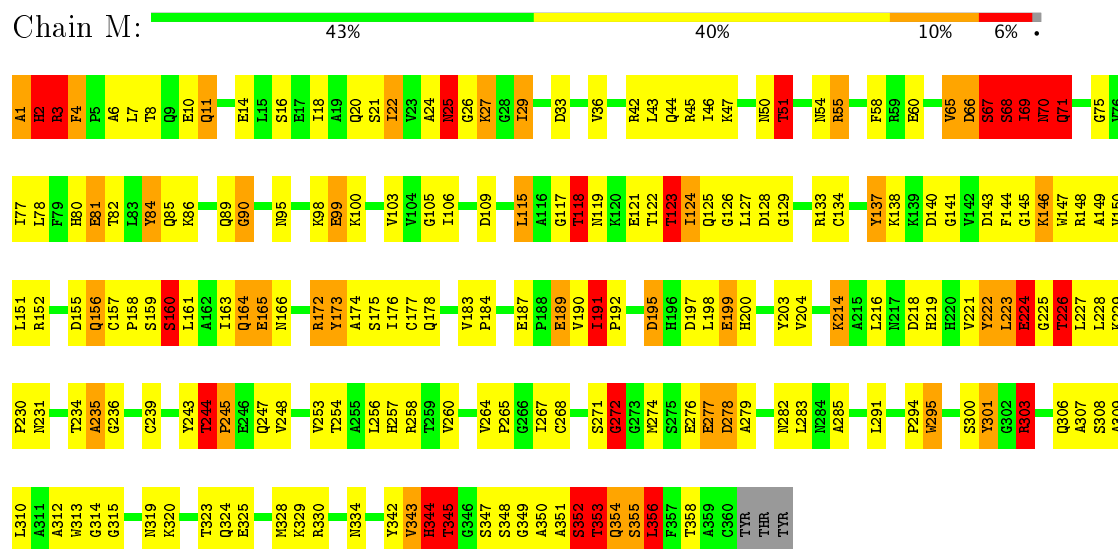


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

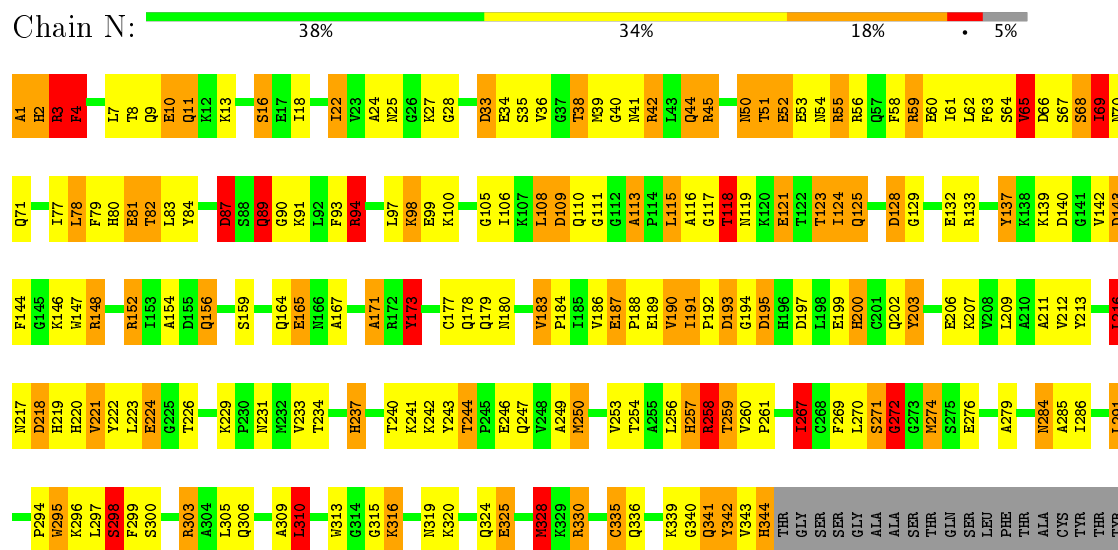
Chain L: 32% 40% 19% 5%



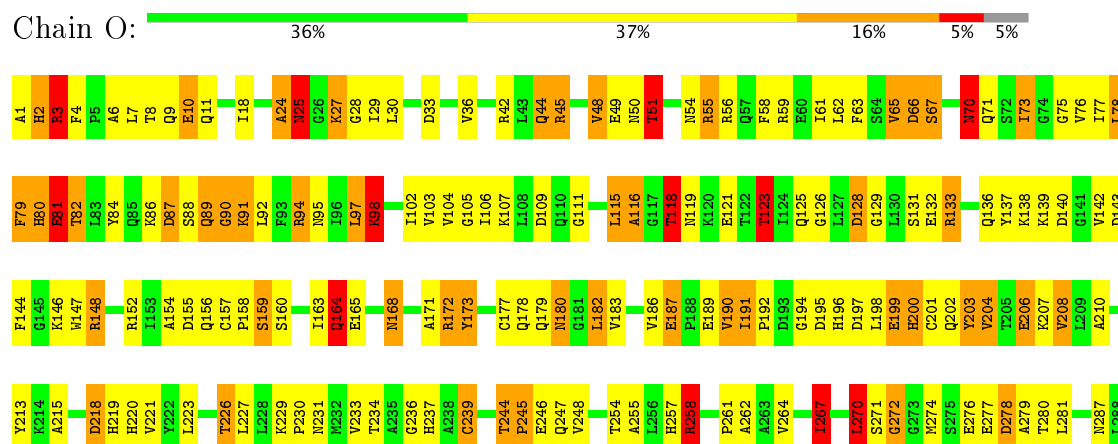
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



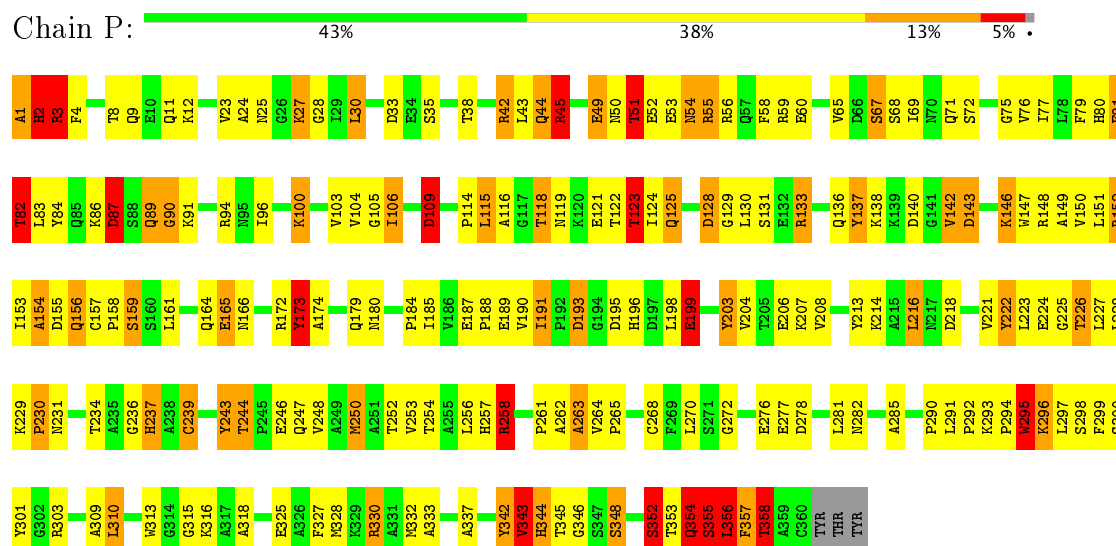
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



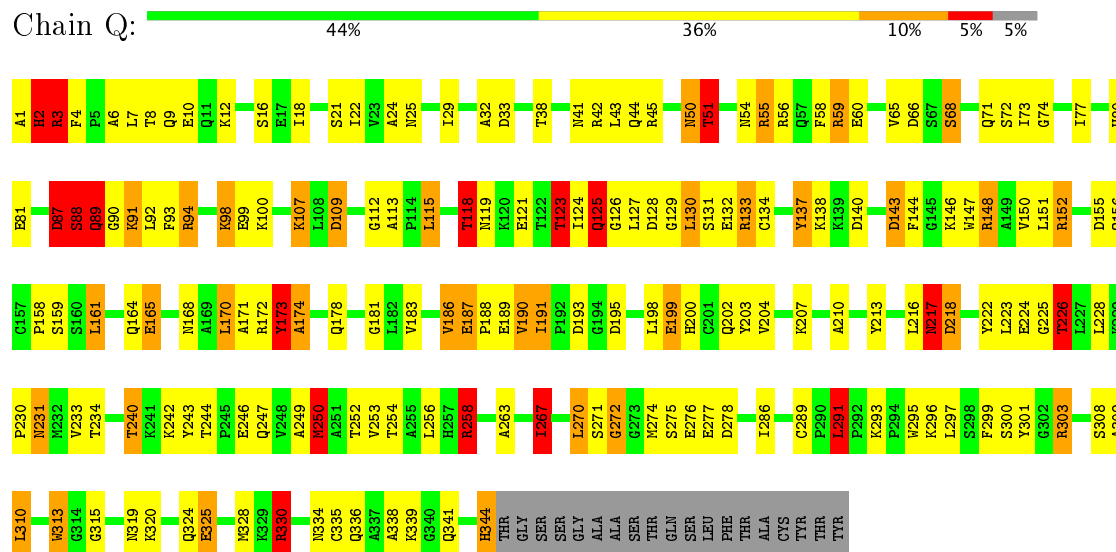
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



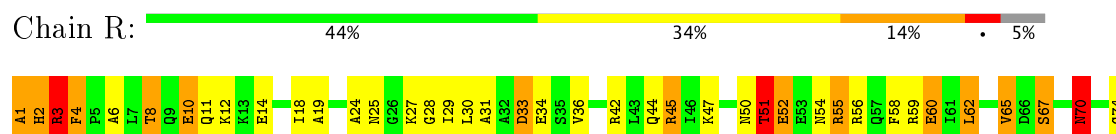
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B



A309	A310	A311	A312	A313	A314	A315	A316	E321	A322	T323	F327	M328	K329	R330	A333	Y342	V343	H344	THR	GLY	SER	SER	GLY	GLY	ALA	ALA	SER	THR	GLN	SER	SER	LEU	PHE	THR	THR	ALA	CYS	TYR	THR	TYR												
K229	P230	M231	M232	V233	T234	R237	A238	C239	T240	K241	K242	Y243	T244	E246	Q247	M250	T254	H257	R258	V264	P265	G266	T267	C268	S271	G272	G273	M274	S275	E276	E277	D278	A279	T280	C289	P290	L291	P292	K293	P294	M295	F299	S300	Y301	G302	R303	Q306	A307	S308			
G75	V76	H80	E81	K86	D87	S88	S88	S88	S88	G90	R94	N95	K98	E99	K100	G101	I102	K107	L108	D109	G112	A113	P114	L115	T118	M119	K120	E121	T122	T123	I124	Q125	G126	L127	D128	G129	L130	S131	E132	R133	C134	Y137	K138	K139	D140	G141	V142	D143	K146	W147	R148	A149
R152	I153	A154	D155	Q156	S159	S160	L161	A162	I163	Q164	E165	A171	R172	Y173	I176	C177	Q178	V183	V190	I191	P192	D193	G194	D195	H196	D197	L198	E199	H200	C201	Q202	Y203	K207	V208	Y212	Y213	R214	A215	L216	M217	D218	H219	R220	V221	Y222	L223	E224	G225	T226	L227	L228	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	291.10 Å 489.84 Å 103.36 Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50	Depositor
% Data completeness (in resolution range)	71.0 (29.00-2.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49278	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.13	2/2776 (0.1%)	2.86	194/3754 (5.2%)
1	B	1.31	11/2696 (0.4%)	2.80	253/3645 (6.9%)
1	C	1.01	0/2680	2.67	155/3624 (4.3%)
1	D	1.28	13/2746 (0.5%)	2.90	248/3713 (6.7%)
1	E	1.08	7/2732 (0.3%)	2.93	189/3694 (5.1%)
1	F	1.03	4/2719 (0.1%)	2.80	183/3677 (5.0%)
1	G	1.03	1/2673 (0.0%)	2.64	169/3614 (4.7%)
1	H	1.01	4/2758 (0.1%)	2.67	175/3729 (4.7%)
1	I	1.08	3/2673 (0.1%)	2.70	210/3614 (5.8%)
1	J	1.06	2/2746 (0.1%)	2.93	184/3713 (5.0%)
1	K	1.06	2/2731 (0.1%)	2.68	163/3693 (4.4%)
1	L	1.06	1/2673 (0.0%)	2.54	160/3614 (4.4%)
1	M	1.06	5/2776 (0.2%)	2.62	170/3754 (4.5%)
1	N	1.06	2/2673 (0.1%)	2.86	180/3614 (5.0%)
1	O	1.07	0/2673	2.49	155/3614 (4.3%)
1	P	1.04	1/2776 (0.0%)	2.69	168/3754 (4.5%)
1	Q	1.02	2/2673 (0.1%)	2.80	158/3614 (4.4%)
1	R	1.04	1/2673 (0.0%)	2.66	156/3614 (4.3%)
All	All	1.08	61/48847 (0.1%)	2.74	3270/66048 (5.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	13
1	C	0	6
1	D	0	13
1	E	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	4
1	G	0	8
1	H	0	7
1	I	0	11
1	J	0	4
1	K	0	6
1	L	0	6
1	M	0	8
1	N	0	6
1	O	0	5
1	P	0	6
1	Q	0	6
1	R	0	10
All	All	0	133

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	187	GLU	CD-OE1	-12.36	1.12	1.25
1	I	67	SER	CA-CB	9.89	1.67	1.52
1	D	187	GLU	CD-OE2	9.61	1.36	1.25
1	J	25	ASN	N-CA	8.98	1.64	1.46
1	E	25	ASN	N-CA	8.96	1.64	1.46
1	B	213	TYR	C-O	-8.91	1.06	1.23
1	P	159	SER	CB-OG	8.85	1.53	1.42
1	B	1	ALA	N-CA	8.81	1.64	1.46
1	E	89	GLN	CB-CG	8.80	1.76	1.52
1	A	308	SER	CB-OG	-8.77	1.30	1.42
1	D	70	ASN	CA-CB	8.21	1.74	1.53
1	H	25	ASN	N-CA	8.16	1.62	1.46
1	B	214	LYS	N-CA	-7.83	1.30	1.46
1	D	25	ASN	N-CA	7.54	1.61	1.46
1	Q	90	GLY	N-CA	7.08	1.56	1.46
1	R	25	ASN	N-CA	7.03	1.60	1.46
1	K	349	GLY	N-CA	6.98	1.56	1.46
1	D	189	GLU	CD-OE2	-6.90	1.18	1.25
1	K	177	CYS	CB-SG	-6.89	1.70	1.82
1	E	159	SER	CB-OG	6.88	1.51	1.42
1	D	212	VAL	C-O	6.65	1.35	1.23
1	D	189	GLU	CD-OE1	6.50	1.32	1.25
1	M	70	ASN	N-CA	-6.49	1.33	1.46
1	M	25	ASN	N-CA	6.48	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	214	LYS	N-CA	6.44	1.59	1.46
1	B	298	SER	CA-CB	6.42	1.62	1.52
1	A	258	ARG	CZ-NH2	6.38	1.41	1.33
1	B	215	ALA	N-CA	-6.27	1.33	1.46
1	B	25	ASN	N-CA	6.25	1.58	1.46
1	G	302	GLY	N-CA	6.25	1.55	1.46
1	I	67	SER	N-CA	-6.16	1.34	1.46
1	M	157	CYS	CB-SG	-6.16	1.71	1.82
1	B	21	SER	CA-CB	6.14	1.62	1.52
1	B	215	ALA	C-O	6.10	1.34	1.23
1	Q	25	ASN	N-CA	6.07	1.58	1.46
1	B	214	LYS	C-O	5.99	1.34	1.23
1	D	87	ASP	CA-CB	5.94	1.67	1.53
1	E	89	GLN	CA-C	5.94	1.68	1.52
1	H	70	ASN	CA-CB	5.88	1.68	1.53
1	F	94	ARG	CD-NE	-5.85	1.36	1.46
1	L	25	ASN	N-CA	5.83	1.58	1.46
1	F	25	ASN	N-CA	5.81	1.57	1.46
1	D	273	GLY	N-CA	5.62	1.54	1.46
1	M	65	VAL	CB-CG1	-5.58	1.41	1.52
1	H	24	ALA	C-O	5.58	1.33	1.23
1	E	94	ARG	CD-NE	-5.53	1.37	1.46
1	F	21	SER	CB-OG	5.45	1.49	1.42
1	N	59	ARG	CD-NE	5.43	1.55	1.46
1	H	94	ARG	NE-CZ	-5.41	1.26	1.33
1	I	266	GLY	N-CA	5.39	1.54	1.46
1	J	289	CYS	CB-SG	-5.37	1.73	1.81
1	D	215	ALA	C-O	-5.28	1.13	1.23
1	F	68	SER	CB-OG	-5.27	1.35	1.42
1	D	152	ARG	CB-CG	-5.26	1.38	1.52
1	N	148	ARG	NE-CZ	-5.25	1.26	1.33
1	D	211	ALA	C-O	-5.16	1.13	1.23
1	M	68	SER	CA-CB	-5.14	1.45	1.52
1	B	213	TYR	CG-CD2	5.11	1.45	1.39
1	E	165	GLU	CD-OE2	5.07	1.31	1.25
1	E	189	GLU	CD-OE1	5.04	1.31	1.25
1	B	221	VAL	N-CA	-5.02	1.36	1.46

All (3270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	42	ARG	NE-CZ-NH2	58.27	149.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH1	54.61	147.61	120.30
1	Q	258	ARG	NE-CZ-NH1	48.20	144.40	120.30
1	D	258	ARG	NE-CZ-NH1	42.36	141.48	120.30
1	L	258	ARG	NE-CZ-NH2	-41.78	99.41	120.30
1	P	330	ARG	NE-CZ-NH2	40.16	140.38	120.30
1	J	94	ARG	CD-NE-CZ	39.36	178.70	123.60
1	C	3	ARG	CD-NE-CZ	37.58	176.21	123.60
1	F	330	ARG	NE-CZ-NH1	-36.87	101.87	120.30
1	E	94	ARG	CD-NE-CZ	36.67	174.94	123.60
1	P	330	ARG	NE-CZ-NH1	-35.62	102.49	120.30
1	K	258	ARG	NE-CZ-NH1	35.05	137.83	120.30
1	Q	172	ARG	CD-NE-CZ	34.74	172.24	123.60
1	F	258	ARG	NE-CZ-NH2	-34.19	103.20	120.30
1	E	258	ARG	NE-CZ-NH1	34.10	137.35	120.30
1	N	303	ARG	NE-CZ-NH1	-33.95	103.33	120.30
1	J	42	ARG	NE-CZ-NH1	-33.40	103.60	120.30
1	A	258	ARG	NE-CZ-NH2	-32.95	103.83	120.30
1	J	258	ARG	NE-CZ-NH1	32.47	136.54	120.30
1	E	148	ARG	CD-NE-CZ	32.20	168.68	123.60
1	F	330	ARG	NE-CZ-NH2	32.01	136.31	120.30
1	Q	330	ARG	NE-CZ-NH2	31.32	135.96	120.30
1	J	258	ARG	NE-CZ-NH2	-31.18	104.71	120.30
1	R	148	ARG	CD-NE-CZ	31.08	167.11	123.60
1	F	94	ARG	CD-NE-CZ	30.68	166.56	123.60
1	D	258	ARG	NE-CZ-NH2	-30.43	105.08	120.30
1	G	330	ARG	NE-CZ-NH2	29.82	135.21	120.30
1	Q	258	ARG	NE-CZ-NH2	-29.80	105.40	120.30
1	C	258	ARG	NE-CZ-NH1	29.55	135.07	120.30
1	N	330	ARG	NE-CZ-NH2	29.47	135.03	120.30
1	L	258	ARG	NE-CZ-NH1	29.13	134.87	120.30
1	N	303	ARG	NE-CZ-NH2	29.11	134.85	120.30
1	M	3	ARG	CD-NE-CZ	27.48	162.07	123.60
1	G	94	ARG	CD-NE-CZ	26.48	160.67	123.60
1	R	258	ARG	NE-CZ-NH1	26.09	133.35	120.30
1	I	152	ARG	NE-CZ-NH2	26.03	133.31	120.30
1	R	258	ARG	CD-NE-CZ	26.01	160.01	123.60
1	M	68	SER	N-CA-CB	25.00	148.00	110.50
1	N	258	ARG	NE-CZ-NH1	24.90	132.75	120.30
1	H	94	ARG	CD-NE-CZ	24.72	158.21	123.60
1	N	152	ARG	NE-CZ-NH1	-24.15	108.22	120.30
1	K	330	ARG	NE-CZ-NH1	-24.14	108.23	120.30
1	A	148	ARG	CD-NE-CZ	24.04	157.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	89	GLN	CA-CB-CG	-23.37	61.98	113.40
1	N	258	ARG	CD-NE-CZ	23.14	156.00	123.60
1	A	330	ARG	NE-CZ-NH2	23.13	131.87	120.30
1	Q	87	ASP	CB-CG-OD2	-23.03	97.57	118.30
1	H	1	ALA	C-N-CA	22.70	178.46	121.70
1	F	258	ARG	NE-CZ-NH1	22.64	131.62	120.30
1	N	3	ARG	NE-CZ-NH1	-22.61	108.99	120.30
1	E	258	ARG	NE-CZ-NH2	-22.59	109.00	120.30
1	G	87	ASP	CB-CG-OD2	22.41	138.47	118.30
1	F	94	ARG	NE-CZ-NH1	-22.40	109.10	120.30
1	M	352	SER	C-N-CA	22.24	177.29	121.70
1	B	203	TYR	CB-CG-CD1	-22.22	107.67	121.00
1	G	148	ARG	NE-CZ-NH1	-22.19	109.21	120.30
1	D	1	ALA	C-N-CA	22.15	177.08	121.70
1	K	330	ARG	NE-CZ-NH2	22.14	131.37	120.30
1	E	148	ARG	NE-CZ-NH2	-21.78	109.41	120.30
1	J	172	ARG	NE-CZ-NH1	21.74	131.17	120.30
1	F	352	SER	C-N-CA	21.34	175.04	121.70
1	R	330	ARG	NE-CZ-NH2	21.31	130.96	120.30
1	H	344	HIS	C-N-CA	21.12	174.50	121.70
1	J	330	ARG	NE-CZ-NH1	-20.97	109.81	120.30
1	G	87	ASP	CB-CG-OD1	-20.85	99.54	118.30
1	N	148	ARG	CD-NE-CZ	20.84	152.78	123.60
1	E	89	GLN	OE1-CD-NE2	20.72	169.55	121.90
1	H	42	ARG	NE-CZ-NH1	-20.62	109.99	120.30
1	P	172	ARG	NE-CZ-NH2	-20.60	110.00	120.30
1	E	165	GLU	OE1-CD-OE2	20.54	147.95	123.30
1	E	89	GLN	N-CA-CB	-20.22	74.21	110.60
1	R	2	HIS	CA-CB-CG	20.20	147.94	113.60
1	R	94	ARG	NE-CZ-NH1	-20.05	110.28	120.30
1	K	152	ARG	NE-CZ-NH1	-19.93	110.33	120.30
1	K	133	ARG	NE-CZ-NH1	-19.72	110.44	120.30
1	C	87	ASP	CB-CG-OD2	-19.63	100.63	118.30
1	A	3	ARG	CD-NE-CZ	19.50	150.91	123.60
1	A	140	ASP	CB-CG-OD2	19.47	135.82	118.30
1	P	258	ARG	NE-CZ-NH2	19.46	130.03	120.30
1	B	203	TYR	CB-CG-CD2	19.34	132.61	121.00
1	M	356	LEU	O-C-N	-19.32	91.79	122.70
1	A	356	LEU	C-N-CA	19.26	169.85	121.70
1	E	89	GLN	CB-CA-C	-19.24	71.92	110.40
1	P	152	ARG	CB-CG-CD	19.14	161.37	111.60
1	H	42	ARG	NE-CZ-NH2	18.93	129.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	ARG	CD-NE-CZ	18.92	150.09	123.60
1	Q	87	ASP	CB-CG-OD1	18.76	135.18	118.30
1	R	344	HIS	CA-CB-CG	18.73	145.43	113.60
1	R	94	ARG	CD-NE-CZ	18.66	149.73	123.60
1	D	45	ARG	NE-CZ-NH2	-18.47	111.06	120.30
1	L	56	ARG	NE-CZ-NH2	-18.45	111.07	120.30
1	O	148	ARG	NE-CZ-NH2	18.36	129.48	120.30
1	E	3	ARG	CD-NE-CZ	18.24	149.13	123.60
1	N	94	ARG	CD-NE-CZ	18.24	149.13	123.60
1	E	133	ARG	NE-CZ-NH1	-18.18	111.21	120.30
1	R	55	ARG	NE-CZ-NH2	-18.07	111.27	120.30
1	A	133	ARG	NE-CZ-NH2	-17.98	111.31	120.30
1	K	148	ARG	NE-CZ-NH1	17.95	129.28	120.30
1	C	1	ALA	C-N-CA	17.93	166.51	121.70
1	M	172	ARG	NE-CZ-NH2	-17.88	111.36	120.30
1	I	330	ARG	NE-CZ-NH2	17.82	129.21	120.30
1	Q	56	ARG	NE-CZ-NH1	17.67	129.13	120.30
1	C	152	ARG	NE-CZ-NH2	17.63	129.11	120.30
1	O	133	ARG	NE-CZ-NH1	-17.57	111.51	120.30
1	E	88	SER	CA-C-N	17.56	155.83	117.20
1	K	94	ARG	NE-CZ-NH2	-17.56	111.52	120.30
1	P	133	ARG	NE-CZ-NH1	-17.41	111.60	120.30
1	J	59	ARG	NE-CZ-NH1	17.40	129.00	120.30
1	H	303	ARG	NE-CZ-NH1	-17.24	111.68	120.30
1	K	347	SER	C-N-CA	17.20	164.71	121.70
1	Q	133	ARG	NE-CZ-NH2	-17.19	111.70	120.30
1	E	88	SER	O-C-N	-17.05	95.42	122.70
1	F	195	ASP	CB-CG-OD1	-17.04	102.96	118.30
1	I	42	ARG	NE-CZ-NH2	16.97	128.78	120.30
1	P	94	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	P	195	ASP	CB-CG-OD2	16.69	133.32	118.30
1	G	65	VAL	CA-C-N	16.68	153.90	117.20
1	K	133	ARG	CD-NE-CZ	-16.68	100.25	123.60
1	C	330	ARG	NE-CZ-NH2	16.63	128.62	120.30
1	D	199	GLU	CA-CB-CG	16.46	149.62	113.40
1	C	133	ARG	NE-CZ-NH2	16.43	128.51	120.30
1	O	94	ARG	NE-CZ-NH2	16.35	128.47	120.30
1	C	94	ARG	NE-CZ-NH1	16.33	128.47	120.30
1	H	258	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	Q	303	ARG	CG-CD-NE	16.12	145.65	111.80
1	Q	267	ILE	CA-CB-CG2	16.08	143.06	110.90
1	N	56	ARG	NE-CZ-NH2	-15.94	112.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	ASP	CA-C-N	15.92	152.23	117.20
1	D	70	ASN	CB-CA-C	-15.92	78.57	110.40
1	K	42	ARG	NE-CZ-NH2	15.80	128.20	120.30
1	N	152	ARG	NE-CZ-NH2	15.74	128.17	120.30
1	A	140	ASP	CB-CG-OD1	-15.68	104.19	118.30
1	D	191	ILE	CA-CB-CG2	15.57	142.03	110.90
1	L	3	ARG	NE-CZ-NH2	15.57	128.08	120.30
1	M	199	GLU	CA-CB-CG	15.54	147.58	113.40
1	J	148	ARG	CD-NE-CZ	15.52	145.33	123.60
1	G	267	ILE	CA-CB-CG2	15.43	141.77	110.90
1	N	330	ARG	NE-CZ-NH1	-15.39	112.60	120.30
1	P	203	TYR	CB-CG-CD2	15.39	130.23	121.00
1	C	59	ARG	NE-CZ-NH1	-15.35	112.63	120.30
1	K	258	ARG	CD-NE-CZ	15.27	144.97	123.60
1	C	330	ARG	NE-CZ-NH1	-15.24	112.68	120.30
1	B	87	ASP	CA-C-N	15.21	150.65	117.20
1	Q	243	TYR	CB-CG-CD1	15.19	130.11	121.00
1	H	56	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	M	330	ARG	NE-CZ-NH1	-15.12	112.74	120.30
1	E	148	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	C	56	ARG	NE-CZ-NH2	-15.04	112.78	120.30
1	D	42	ARG	NE-CZ-NH2	15.03	127.81	120.30
1	K	33	ASP	CB-CG-OD1	-14.97	104.83	118.30
1	M	45	ARG	NE-CZ-NH2	-14.93	112.84	120.30
1	E	89	GLN	CG-CD-OE1	-14.91	91.78	121.60
1	N	191	ILE	CA-CB-CG2	14.88	140.67	110.90
1	D	164	GLN	CA-CB-CG	14.88	146.13	113.40
1	E	94	ARG	NE-CZ-NH1	-14.83	112.88	120.30
1	I	55	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	J	1	ALA	CB-CA-C	14.72	132.18	110.10
1	I	67	SER	CB-CA-C	-14.71	82.16	110.10
1	O	203	TYR	CB-CG-CD1	-14.68	112.19	121.00
1	M	1	ALA	CB-CA-C	14.61	132.01	110.10
1	N	3	ARG	NE-CZ-NH2	14.59	127.59	120.30
1	B	94	ARG	CD-NE-CZ	14.59	144.02	123.60
1	A	357	PHE	CB-CG-CD1	-14.57	110.60	120.80
1	H	191	ILE	CA-CB-CG2	14.57	140.04	110.90
1	M	69	ILE	CB-CA-C	14.50	140.61	111.60
1	F	140	ASP	CB-CG-OD1	-14.48	105.27	118.30
1	B	3	ARG	NE-CZ-NH1	14.48	127.54	120.30
1	Q	243	TYR	CB-CG-CD2	-14.44	112.34	121.00
1	I	191	ILE	CA-CB-CG2	14.43	139.76	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	330	ARG	NE-CZ-NH1	-14.40	113.10	120.30
1	M	258	ARG	NE-CZ-NH1	14.37	127.49	120.30
1	E	1	ALA	C-N-CA	14.34	157.55	121.70
1	B	213	TYR	CB-CG-CD2	-14.34	112.40	121.00
1	I	152	ARG	NE-CZ-NH1	-14.31	113.14	120.30
1	B	195	ASP	CB-CG-OD2	14.29	131.16	118.30
1	R	303	ARG	CD-NE-CZ	-14.27	103.62	123.60
1	O	94	ARG	NE-CZ-NH1	-14.24	113.18	120.30
1	H	165	GLU	OE1-CD-OE2	14.20	140.34	123.30
1	F	172	ARG	NE-CZ-NH1	-14.19	113.20	120.30
1	P	140	ASP	CB-CG-OD2	14.19	131.07	118.30
1	G	258	ARG	NE-CZ-NH1	14.09	127.35	120.30
1	N	258	ARG	NE-CZ-NH2	-14.07	113.27	120.30
1	J	133	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	C	152	ARG	NE-CZ-NH1	-14.02	113.29	120.30
1	C	87	ASP	CB-CA-C	-13.98	82.43	110.40
1	K	109	ASP	CB-CG-OD1	13.92	130.83	118.30
1	H	172	ARG	NE-CZ-NH2	-13.89	113.35	120.30
1	F	42	ARG	NE-CZ-NH2	13.87	127.24	120.30
1	K	152	ARG	NE-CZ-NH2	13.79	127.20	120.30
1	D	303	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	C	258	ARG	CD-NE-CZ	13.74	142.84	123.60
1	K	45	ARG	NE-CZ-NH2	-13.73	113.43	120.30
1	C	173	TYR	CB-CG-CD1	13.69	129.21	121.00
1	D	87	ASP	CB-CG-OD1	-13.69	105.98	118.30
1	F	133	ARG	NE-CZ-NH1	-13.69	113.46	120.30
1	B	42	ARG	NE-CZ-NH2	13.65	127.13	120.30
1	C	173	TYR	CB-CG-CD2	-13.65	112.81	121.00
1	M	303	ARG	CD-NE-CZ	13.65	142.71	123.60
1	I	87	ASP	CB-CG-OD1	-13.64	106.02	118.30
1	C	132	GLU	OE1-CD-OE2	-13.61	106.97	123.30
1	I	2	HIS	CA-CB-CG	13.59	136.70	113.60
1	K	88	SER	CA-C-N	13.58	147.08	117.20
1	J	45	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	M	70	ASN	CB-CA-C	-13.49	83.42	110.40
1	I	206	GLU	OE1-CD-OE2	-13.47	107.13	123.30
1	E	203	TYR	CB-CG-CD1	-13.43	112.94	121.00
1	K	195	ASP	CB-CG-OD1	-13.42	106.22	118.30
1	J	109	ASP	CB-CG-OD2	-13.40	106.24	118.30
1	D	148	ARG	NE-CZ-NH1	-13.40	113.60	120.30
1	F	195	ASP	CB-CG-OD2	13.36	130.32	118.30
1	F	243	TYR	CB-CG-CD2	-13.35	112.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	165	GLU	OE1-CD-OE2	13.34	139.30	123.30
1	M	55	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	D	203	TYR	CB-CG-CD2	13.28	128.97	121.00
1	I	66	ASP	CB-CG-OD1	13.24	130.22	118.30
1	F	148	ARG	CD-NE-CZ	13.23	142.12	123.60
1	N	87	ASP	CB-CG-OD2	-13.22	106.40	118.30
1	N	3	ARG	C-N-CA	13.22	154.75	121.70
1	N	87	ASP	CB-CA-C	-13.22	83.97	110.40
1	P	193	ASP	CB-CG-OD1	13.20	130.18	118.30
1	A	133	ARG	NH1-CZ-NH2	13.19	133.91	119.40
1	Q	165	GLU	OE1-CD-OE2	13.19	139.13	123.30
1	H	258	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	J	70	ASN	CB-CA-C	-13.06	84.27	110.40
1	N	3	ARG	CA-C-O	13.06	147.52	120.10
1	A	258	ARG	CD-NE-CZ	13.04	141.85	123.60
1	R	1	ALA	CB-CA-C	13.04	129.65	110.10
1	F	87	ASP	CB-CG-OD2	13.00	130.00	118.30
1	A	330	ARG	NE-CZ-NH1	-12.97	113.81	120.30
1	G	191	ILE	CA-CB-CG2	12.95	136.79	110.90
1	A	303	ARG	CD-NE-CZ	-12.94	105.48	123.60
1	H	303	ARG	NE-CZ-NH2	12.94	126.77	120.30
1	A	358	THR	N-CA-CB	12.94	134.88	110.30
1	M	68	SER	C-N-CA	-12.94	89.36	121.70
1	I	67	SER	N-CA-CB	-12.92	91.11	110.50
1	G	133	ARG	NE-CZ-NH1	-12.87	113.86	120.30
1	N	132	GLU	OE1-CD-OE2	-12.87	107.86	123.30
1	Q	140	ASP	CB-CG-OD1	-12.85	106.74	118.30
1	P	148	ARG	NE-CZ-NH1	12.83	126.72	120.30
1	I	303	ARG	CD-NE-CZ	12.81	141.53	123.60
1	M	68	SER	CB-CA-C	-12.80	85.79	110.10
1	N	148	ARG	NE-CZ-NH2	-12.77	113.91	120.30
1	H	87	ASP	CB-CG-OD2	12.71	129.74	118.30
1	A	87	ASP	CB-CA-C	-12.68	85.04	110.40
1	D	195	ASP	CB-CG-OD1	-12.68	106.89	118.30
1	P	218	ASP	CB-CG-OD1	12.67	129.70	118.30
1	E	66	ASP	CA-C-N	12.64	145.01	117.20
1	P	45	ARG	NE-CZ-NH2	-12.61	113.99	120.30
1	P	189	GLU	OE1-CD-OE2	-12.61	108.17	123.30
1	P	152	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	A	203	TYR	CB-CG-CD2	12.60	128.56	121.00
1	E	94	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	M	172	ARG	NE-CZ-NH1	12.56	126.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	94	ARG	NE-CZ-NH1	12.55	126.57	120.30
1	N	3	ARG	CD-NE-CZ	12.55	141.17	123.60
1	H	330	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	E	89	GLN	CG-CD-NE2	-12.53	86.63	116.70
1	N	1	ALA	N-CA-CB	12.51	127.62	110.10
1	H	55	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	J	172	ARG	NE-CZ-NH2	-12.47	114.07	120.30
1	Q	66	ASP	CB-CG-OD1	12.45	129.50	118.30
1	J	203	TYR	CB-CG-CD1	-12.43	113.54	121.00
1	H	70	ASN	CB-CA-C	-12.43	85.55	110.40
1	A	94	ARG	NE-CZ-NH2	-12.39	114.10	120.30
1	M	303	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	H	67	SER	N-CA-CB	12.38	129.07	110.50
1	Q	195	ASP	CB-CG-OD2	12.38	129.44	118.30
1	E	94	ARG	NH1-CZ-NH2	12.37	133.01	119.40
1	D	356	LEU	CA-C-O	12.33	145.99	120.10
1	F	56	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	152	ARG	NE-CZ-NH1	-12.31	114.14	120.30
1	E	88	SER	CA-C-O	-12.28	94.30	120.10
1	K	258	ARG	NH1-CZ-NH2	-12.28	105.89	119.40
1	E	347	SER	CB-CA-C	-12.26	86.82	110.10
1	K	133	ARG	NH1-CZ-NH2	12.21	132.84	119.40
1	P	56	ARG	NE-CZ-NH2	12.21	126.41	120.30
1	N	3	ARG	O-C-N	-12.20	103.17	122.70
1	P	87	ASP	CB-CA-C	-12.19	86.02	110.40
1	I	70	ASN	CB-CG-OD1	12.16	145.91	121.60
1	H	303	ARG	CD-NE-CZ	-12.13	106.62	123.60
1	I	59	ARG	NE-CZ-NH1	-12.11	114.25	120.30
1	H	87	ASP	CB-CG-OD1	-12.10	107.41	118.30
1	N	173	TYR	CB-CG-CD2	-12.07	113.76	121.00
1	M	69	ILE	N-CA-CB	-12.05	83.09	110.80
1	O	94	ARG	CD-NE-CZ	11.98	140.37	123.60
1	C	137	TYR	CB-CG-CD1	11.89	128.14	121.00
1	J	258	ARG	CD-NE-CZ	11.88	140.24	123.60
1	F	59	ARG	NE-CZ-NH2	11.88	126.24	120.30
1	M	258	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	F	56	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	J	191	ILE	CA-CB-CG2	11.83	134.57	110.90
1	A	87	ASP	CB-CG-OD1	-11.83	107.66	118.30
1	E	226	THR	CA-CB-CG2	11.83	128.96	112.40
1	G	133	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	G	94	ARG	NE-CZ-NH1	-11.79	114.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	128	ASP	CB-CG-OD1	-11.78	107.70	118.30
1	I	172	ARG	NE-CZ-NH1	-11.76	114.42	120.30
1	P	133	ARG	CD-NE-CZ	-11.73	107.18	123.60
1	R	42	ARG	NE-CZ-NH1	-11.71	114.45	120.30
1	R	148	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	N	59	ARG	CD-NE-CZ	-11.66	107.28	123.60
1	D	66	ASP	CB-CG-OD2	11.65	128.78	118.30
1	G	70	ASN	CB-CA-C	-11.65	87.10	110.40
1	B	195	ASP	CB-CG-OD1	-11.64	107.82	118.30
1	E	55	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	Q	195	ASP	CB-CG-OD1	-11.64	107.82	118.30
1	M	203	TYR	CB-CG-CD2	11.62	127.97	121.00
1	A	128	ASP	CB-CG-OD1	-11.62	107.85	118.30
1	Q	330	ARG	NH1-CZ-NH2	-11.59	106.65	119.40
1	Q	94	ARG	NE-CZ-NH2	11.59	126.09	120.30
1	E	344	HIS	C-N-CA	11.59	150.67	121.70
1	Q	68	SER	N-CA-CB	-11.59	93.12	110.50
1	R	258	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	H	2	HIS	CA-CB-CG	11.55	133.23	113.60
1	Q	55	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	B	197	ASP	CB-CG-OD1	11.54	128.68	118.30
1	M	191	ILE	CA-CB-CG2	11.51	133.92	110.90
1	G	65	VAL	O-C-N	-11.51	104.29	122.70
1	G	66	ASP	N-CA-CB	11.50	131.31	110.60
1	C	3	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	B	3	ARG	CD-NE-CZ	11.47	139.66	123.60
1	P	55	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	M	3	ARG	NE-CZ-NH2	11.43	126.02	120.30
1	E	258	ARG	CD-NE-CZ	11.41	139.58	123.60
1	O	258	ARG	NE-CZ-NH1	-11.41	114.60	120.30
1	G	172	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	R	165	GLU	OE1-CD-OE2	11.37	136.94	123.30
1	L	262	ALA	N-CA-CB	-11.32	94.25	110.10
1	J	42	ARG	NH1-CZ-NH2	-11.31	106.96	119.40
1	Q	42	ARG	CD-NE-CZ	11.31	139.43	123.60
1	I	148	ARG	CD-NE-CZ	11.29	139.40	123.60
1	K	243	TYR	CB-CG-CD2	11.27	127.76	121.00
1	M	195	ASP	CB-CG-OD1	-11.26	108.16	118.30
1	M	352	SER	O-C-N	-11.25	104.70	122.70
1	M	42	ARG	CD-NE-CZ	11.25	139.35	123.60
1	R	140	ASP	CB-CG-OD2	-11.23	108.19	118.30
1	F	10	GLU	CA-CB-CG	11.23	138.11	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH2	11.23	125.91	120.30
1	H	66	ASP	O-C-N	-11.23	104.74	122.70
1	B	191	ILE	CA-CB-CG2	11.22	133.34	110.90
1	G	133	ARG	NH1-CZ-NH2	11.20	131.72	119.40
1	F	191	ILE	CA-CB-CG2	11.18	133.26	110.90
1	E	27	LYS	CD-CE-NZ	11.17	137.39	111.70
1	P	42	ARG	NE-CZ-NH2	11.13	125.86	120.30
1	L	33	ASP	CB-CG-OD2	-11.11	108.30	118.30
1	Q	3	ARG	O-C-N	-11.10	104.93	122.70
1	K	87	ASP	CB-CG-OD1	11.10	128.29	118.30
1	A	193	ASP	CB-CG-OD1	11.09	128.28	118.30
1	B	90	GLY	CA-C-O	-11.08	100.65	120.60
1	A	133	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	Q	133	ARG	NH1-CZ-NH2	11.05	131.56	119.40
1	N	87	ASP	OD1-CG-OD2	11.04	144.27	123.30
1	B	68	SER	N-CA-CB	-11.03	93.96	110.50
1	A	203	TYR	CB-CG-CD1	-11.02	114.39	121.00
1	P	203	TYR	CB-CG-CD1	-11.01	114.39	121.00
1	P	191	ILE	CA-CB-CG2	10.99	132.88	110.90
1	I	133	ARG	NE-CZ-NH1	10.99	125.79	120.30
1	A	55	ARG	NE-CZ-NH2	10.98	125.79	120.30
1	H	155	ASP	CB-CG-OD2	-10.98	108.42	118.30
1	G	165	GLU	OE1-CD-OE2	10.98	136.47	123.30
1	B	197	ASP	CB-CG-OD2	-10.93	108.47	118.30
1	M	222	TYR	CB-CG-CD2	10.93	127.56	121.00
1	H	55	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	O	187	GLU	OE1-CD-OE2	-10.92	110.20	123.30
1	J	195	ASP	CB-CG-OD1	-10.91	108.48	118.30
1	B	87	ASP	O-C-N	-10.91	105.25	122.70
1	G	70	ASN	N-CA-CB	-10.91	90.97	110.60
1	B	267	ILE	CA-CB-CG2	10.90	132.71	110.90
1	D	215	ALA	CA-C-O	10.89	142.97	120.10
1	E	87	ASP	CB-CG-OD1	10.89	128.10	118.30
1	N	267	ILE	CA-CB-CG2	10.87	132.64	110.90
1	R	152	ARG	NE-CZ-NH1	-10.87	114.86	120.30
1	F	128	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	C	191	ILE	CA-CB-CG2	10.83	132.56	110.90
1	D	70	ASN	CA-CB-CG	-10.83	89.58	113.40
1	I	56	ARG	NE-CZ-NH1	-10.83	114.89	120.30
1	M	67	SER	CA-C-O	10.82	142.82	120.10
1	I	69	ILE	O-C-N	-10.81	105.40	122.70
1	E	67	SER	N-CA-CB	10.81	126.71	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	GLU	CA-CB-CG	10.79	137.14	113.40
1	I	67	SER	N-CA-C	10.75	140.03	111.00
1	G	140	ASP	CB-CG-OD1	-10.72	108.65	118.30
1	G	143	ASP	CB-CG-OD1	-10.72	108.65	118.30
1	M	277	GLU	OE1-CD-OE2	-10.72	110.44	123.30
1	N	218	ASP	CB-CG-OD1	10.71	127.94	118.30
1	E	55	ARG	NE-CZ-NH2	-10.71	114.95	120.30
1	O	303	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	R	148	ARG	NE-CZ-NH2	-10.67	114.96	120.30
1	G	65	VAL	CA-C-O	-10.67	97.69	120.10
1	J	3	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	L	42	ARG	NE-CZ-NH2	10.65	125.63	120.30
1	E	56	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	D	330	ARG	NE-CZ-NH1	-10.63	114.98	120.30
1	G	195	ASP	CB-CG-OD1	-10.63	108.74	118.30
1	F	330	ARG	CD-NE-CZ	-10.62	108.73	123.60
1	K	99	GLU	OE1-CD-OE2	10.62	136.05	123.30
1	D	191	ILE	CA-CB-CG1	-10.59	90.87	111.00
1	E	89	GLN	CB-CG-CD	-10.59	84.06	111.60
1	M	222	TYR	CB-CG-CD1	-10.57	114.66	121.00
1	A	308	SER	CA-CB-OG	10.55	139.70	111.20
1	E	109	ASP	CB-CG-OD1	10.55	127.79	118.30
1	P	195	ASP	CB-CG-OD1	-10.54	108.81	118.30
1	I	94	ARG	CD-NE-CZ	10.51	138.31	123.60
1	D	87	ASP	CB-CA-C	-10.50	89.40	110.40
1	P	94	ARG	NH1-CZ-NH2	10.47	130.92	119.40
1	F	148	ARG	NE-CZ-NH1	-10.47	115.07	120.30
1	F	267	ILE	CA-CB-CG2	10.47	131.84	110.90
1	J	143	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	A	59	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	D	226	THR	CA-CB-CG2	10.40	126.95	112.40
1	M	330	ARG	NE-CZ-NH2	10.37	125.48	120.30
1	B	301	TYR	CB-CG-CD2	10.36	127.21	121.00
1	L	203	TYR	CB-CG-CD1	-10.35	114.79	121.00
1	P	352	SER	N-CA-CB	10.34	126.01	110.50
1	I	56	ARG	CD-NE-CZ	-10.33	109.14	123.60
1	L	87	ASP	CB-CA-C	-10.32	89.75	110.40
1	M	69	ILE	CA-CB-CG2	-10.31	90.27	110.90
1	B	213	TYR	CG-CD2-CE2	-10.31	113.05	121.30
1	B	301	TYR	CB-CG-CD1	-10.29	114.82	121.00
1	Q	89	GLN	CA-C-N	10.29	136.79	116.20
1	E	66	ASP	O-C-N	-10.29	106.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	3	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	F	87	ASP	CB-CG-OD1	-10.28	109.05	118.30
1	M	67	SER	C-N-CA	10.28	147.40	121.70
1	B	303	ARG	CD-NE-CZ	10.28	137.99	123.60
1	B	214	LYS	O-C-N	-10.27	106.26	122.70
1	K	140	ASP	CB-CG-OD2	10.26	127.54	118.30
1	A	199	GLU	OE1-CD-OE2	-10.25	111.00	123.30
1	A	199	GLU	CB-CA-C	10.24	130.88	110.40
1	Q	94	ARG	NE-CZ-NH1	-10.24	115.18	120.30
1	G	3	ARG	NE-CZ-NH1	-10.23	115.19	120.30
1	L	152	ARG	NE-CZ-NH1	-10.23	115.19	120.30
1	Q	303	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	N	59	ARG	NE-CZ-NH1	-10.21	115.19	120.30
1	R	59	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	F	70	ASN	CB-CA-C	-10.14	90.12	110.40
1	P	258	ARG	CB-CG-CD	10.14	137.97	111.60
1	H	59	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	O	195	ASP	CB-CG-OD1	-10.13	109.19	118.30
1	O	152	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	M	152	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	H	133	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	55	ARG	CD-NE-CZ	-10.08	109.49	123.60
1	F	258	ARG	CD-NE-CZ	10.08	137.71	123.60
1	J	217	ASN	CB-CG-OD1	10.08	141.75	121.60
1	E	3	ARG	CA-C-O	10.07	141.25	120.10
1	G	148	ARG	NH1-CZ-NH2	10.07	130.47	119.40
1	D	55	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	D	226	THR	N-CA-CB	-10.06	91.18	110.30
1	I	109	ASP	CB-CG-OD1	-10.06	109.25	118.30
1	E	203	TYR	CB-CG-CD2	10.04	127.02	121.00
1	G	84	TYR	CB-CG-CD1	-10.03	114.98	121.00
1	A	45	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	172	ARG	NE-CZ-NH1	-10.03	115.28	120.30
1	D	152	ARG	O-C-N	10.01	138.72	122.70
1	E	172	ARG	NE-CZ-NH1	-10.01	115.30	120.30
1	J	152	ARG	CD-NE-CZ	-10.00	109.60	123.60
1	N	87	ASP	CB-CG-OD1	-10.00	109.30	118.30
1	Q	191	ILE	CA-CB-CG2	9.98	130.86	110.90
1	G	10	GLU	CA-CB-CG	9.98	135.35	113.40
1	O	197	ASP	CB-CG-OD1	9.98	127.28	118.30
1	D	24	ALA	C-N-CA	-9.96	96.81	121.70
1	A	358	THR	CA-C-O	9.95	141.00	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	352	SER	CA-C-O	9.94	140.97	120.10
1	H	3	ARG	CD-NE-CZ	9.93	137.50	123.60
1	N	195	ASP	CB-CG-OD1	-9.93	109.36	118.30
1	F	55	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	R	70	ASN	CB-CA-C	-9.92	90.57	110.40
1	B	172	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	M	67	SER	N-CA-CB	9.91	125.36	110.50
1	Q	24	ALA	C-N-CA	-9.90	96.96	121.70
1	G	33	ASP	CB-CG-OD2	9.89	127.20	118.30
1	M	149	ALA	N-CA-CB	9.88	123.94	110.10
1	L	94	ARG	CD-NE-CZ	9.88	137.43	123.60
1	J	24	ALA	CA-C-N	9.87	138.91	117.20
1	J	152	ARG	CB-CA-C	-9.86	90.68	110.40
1	J	244	THR	N-CA-CB	-9.86	91.57	110.30
1	A	258	ARG	NH1-CZ-NH2	-9.85	108.57	119.40
1	B	11	GLN	CA-C-O	9.83	140.75	120.10
1	M	67	SER	CA-C-N	-9.83	95.58	117.20
1	D	89	GLN	O-C-N	-9.82	106.50	123.20
1	K	339	LYS	CG-CD-CE	9.82	141.37	111.90
1	K	189	GLU	OE1-CD-OE2	-9.81	111.52	123.30
1	G	123	THR	N-CA-CB	9.81	128.94	110.30
1	D	197	ASP	CB-CG-OD1	9.81	127.13	118.30
1	N	216	LEU	CA-CB-CG	9.81	137.85	115.30
1	R	343	VAL	N-CA-CB	9.80	133.06	111.50
1	D	118	THR	N-CA-CB	-9.77	91.73	110.30
1	H	197	ASP	CB-CG-OD2	9.77	127.10	118.30
1	I	207	LYS	CA-CB-CG	9.77	134.90	113.40
1	D	152	ARG	NE-CZ-NH2	9.77	125.18	120.30
1	J	348	SER	N-CA-CB	9.77	125.15	110.50
1	B	258	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	D	187	GLU	OE1-CD-OE2	9.76	135.01	123.30
1	D	33	ASP	CB-CG-OD2	9.73	127.06	118.30
1	A	148	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	A	33	ASP	CB-CG-OD2	9.71	127.04	118.30
1	D	173	TYR	CB-CG-CD2	-9.71	115.17	121.00
1	R	1	ALA	C-N-CA	9.71	145.97	121.70
1	O	24	ALA	CA-C-N	9.71	138.55	117.20
1	C	137	TYR	CB-CG-CD2	-9.70	115.18	121.00
1	J	152	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	H	3	ARG	CA-C-O	9.68	140.42	120.10
1	H	250	MET	CG-SD-CE	-9.68	84.72	100.20
1	A	42	ARG	NE-CZ-NH2	9.66	125.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	303	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	133	ARG	CD-NE-CZ	-9.66	110.08	123.60
1	D	24	ALA	N-CA-CB	9.66	123.62	110.10
1	K	33	ASP	CB-CG-OD2	9.65	126.99	118.30
1	C	132	GLU	CB-CG-CD	9.65	140.25	114.20
1	D	272	GLY	C-N-CA	-9.64	102.05	122.30
1	D	155	ASP	CB-CG-OD2	9.63	126.96	118.30
1	R	309	ALA	N-CA-CB	9.61	123.56	110.10
1	F	152	ARG	NE-CZ-NH1	-9.61	115.49	120.30
1	L	267	ILE	CA-CB-CG2	9.61	130.12	110.90
1	G	181	GLY	O-C-N	9.60	138.06	122.70
1	R	278	ASP	CB-CG-OD1	9.59	126.93	118.30
1	F	24	ALA	C-N-CA	-9.58	97.74	121.70
1	H	330	ARG	NH1-CZ-NH2	-9.58	108.86	119.40
1	G	330	ARG	NH1-CZ-NH2	-9.57	108.87	119.40
1	O	303	ARG	CD-NE-CZ	9.57	136.99	123.60
1	B	228	LEU	O-C-N	9.56	138.00	122.70
1	I	38	THR	CA-CB-CG2	-9.55	99.03	112.40
1	A	152	ARG	CD-NE-CZ	-9.51	110.29	123.60
1	D	70	ASN	O-C-N	-9.51	107.48	122.70
1	L	24	ALA	C-N-CA	-9.51	97.93	121.70
1	M	68	SER	CA-C-N	-9.51	96.29	117.20
1	C	222	TYR	CB-CG-CD2	9.50	126.70	121.00
1	R	56	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	Q	152	ARG	CD-NE-CZ	-9.49	110.32	123.60
1	J	291	LEU	CA-CB-CG	9.47	137.09	115.30
1	H	3	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	F	140	ASP	CB-CG-OD2	9.46	126.82	118.30
1	C	258	ARG	NH1-CZ-NH2	-9.46	109.00	119.40
1	Q	123	THR	N-CA-CB	9.46	128.27	110.30
1	J	2	HIS	CA-CB-CG	9.45	129.67	113.60
1	H	27	LYS	CD-CE-NZ	9.45	133.43	111.70
1	F	94	ARG	NH1-CZ-NH2	9.44	129.78	119.40
1	I	132	GLU	OE1-CD-OE2	-9.44	111.97	123.30
1	E	133	ARG	NH1-CZ-NH2	9.44	129.78	119.40
1	J	140	ASP	CB-CG-OD2	9.43	126.78	118.30
1	M	303	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	O	257	HIS	O-C-N	9.42	137.77	122.70
1	G	226	THR	N-CA-CB	-9.41	92.42	110.30
1	Q	3	ARG	CG-CD-NE	9.40	131.53	111.80
1	L	253	VAL	CG1-CB-CG2	-9.37	95.91	110.90
1	N	121	GLU	OE1-CD-OE2	-9.36	112.07	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	221	VAL	CA-CB-CG2	-9.35	96.88	110.90
1	D	68	SER	N-CA-CB	-9.33	96.50	110.50
1	E	347	SER	N-CA-CB	9.32	124.48	110.50
1	D	203	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	I	3	ARG	CA-CB-CG	9.30	133.87	113.40
1	E	352	SER	C-N-CA	9.30	144.95	121.70
1	N	330	ARG	CD-NE-CZ	-9.30	110.58	123.60
1	B	212	VAL	O-C-N	9.28	137.56	122.70
1	B	24	ALA	C-N-CA	-9.28	98.50	121.70
1	K	348	SER	CA-C-N	9.27	134.74	116.20
1	G	33	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	N	33	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	G	258	ARG	NH1-CZ-NH2	-9.26	109.22	119.40
1	P	100	LYS	CA-CB-CG	9.23	133.72	113.40
1	I	68	SER	O-C-N	9.22	137.45	122.70
1	C	222	TYR	CB-CG-CD1	-9.21	115.48	121.00
1	H	191	ILE	CA-CB-CG1	-9.20	93.52	111.00
1	O	148	ARG	NE-CZ-NH1	-9.20	115.70	120.30
1	D	215	ALA	CA-C-N	-9.19	96.99	117.20
1	H	171	ALA	N-CA-CB	9.18	122.94	110.10
1	L	203	TYR	CB-CG-CD2	9.18	126.50	121.00
1	N	38	THR	CA-CB-CG2	-9.17	99.56	112.40
1	I	320	LYS	CD-CE-NZ	9.16	132.78	111.70
1	R	3	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	D	88	SER	N-CA-CB	-9.16	96.76	110.50
1	J	132	GLU	OE1-CD-OE2	-9.15	112.32	123.30
1	O	24	ALA	C-N-CA	-9.15	98.82	121.70
1	B	267	ILE	CA-CB-CG1	-9.15	93.61	111.00
1	Q	10	GLU	N-CA-CB	9.13	127.03	110.60
1	H	3	ARG	O-C-N	-9.12	108.10	122.70
1	M	24	ALA	CA-C-N	9.12	137.27	117.20
1	A	292	PRO	O-C-N	-9.12	108.11	122.70
1	B	258	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	E	24	ALA	C-N-CA	-9.12	98.91	121.70
1	A	67	SER	N-CA-CB	-9.11	96.84	110.50
1	O	33	ASP	CB-CG-OD2	-9.11	110.11	118.30
1	M	71	GLN	CA-CB-CG	9.10	133.42	113.40
1	J	267	ILE	CA-CB-CG2	9.09	129.08	110.90
1	B	269	PHE	CG-CD1-CE1	9.08	130.79	120.80
1	K	66	ASP	CB-CG-OD1	9.08	126.47	118.30
1	H	24	ALA	C-N-CA	-9.07	99.01	121.70
1	G	316	LYS	CD-CE-NZ	9.07	132.56	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	10	GLU	CA-CB-CG	9.07	133.36	113.40
1	E	109	ASP	O-C-N	9.04	137.17	122.70
1	K	115	LEU	CB-CG-CD1	9.04	126.38	111.00
1	B	232	MET	CA-CB-CG	9.04	128.66	113.30
1	L	258	ARG	CD-NE-CZ	9.03	136.24	123.60
1	M	199	GLU	CB-CG-CD	9.03	138.57	114.20
1	B	94	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	K	152	ARG	N-CA-CB	9.02	126.83	110.60
1	R	195	ASP	CB-CG-OD1	-9.01	110.19	118.30
1	R	10	GLU	OE1-CD-OE2	-9.01	112.49	123.30
1	J	24	ALA	C-N-CA	-9.00	99.20	121.70
1	D	28	GLY	CA-C-O	9.00	136.79	120.60
1	I	24	ALA	C-N-CA	-9.00	99.21	121.70
1	I	172	ARG	NE-CZ-NH2	9.00	124.80	120.30
1	P	172	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	P	330	ARG	CD-NE-CZ	-8.99	111.02	123.60
1	D	322	ALA	N-CA-CB	-8.98	97.52	110.10
1	P	128	ASP	CB-CG-OD1	-8.97	110.23	118.30
1	Q	59	ARG	NE-CZ-NH2	8.97	124.78	120.30
1	F	66	ASP	CB-CG-OD1	8.97	126.37	118.30
1	R	303	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	N	4	PHE	CB-CG-CD2	-8.96	114.53	120.80
1	H	353	THR	C-N-CA	8.96	144.10	121.70
1	R	24	ALA	C-N-CA	-8.95	99.31	121.70
1	F	303	ARG	CD-NE-CZ	-8.95	111.07	123.60
1	E	3	ARG	CG-CD-NE	8.93	130.55	111.80
1	K	325	GLU	OE1-CD-OE2	8.93	134.02	123.30
1	H	207	LYS	CA-CB-CG	8.92	133.03	113.40
1	K	88	SER	CA-C-O	-8.92	101.37	120.10
1	Q	55	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	G	330	ARG	NE-CZ-NH1	-8.91	115.85	120.30
1	A	152	ARG	N-CA-CB	8.90	126.63	110.60
1	D	66	ASP	OD1-CG-OD2	-8.87	106.44	123.30
1	K	157	CYS	N-CA-CB	-8.88	94.63	110.60
1	O	82	THR	CA-CB-CG2	-8.88	99.97	112.40
1	F	226	THR	N-CA-CB	-8.87	93.44	110.30
1	P	133	ARG	NH1-CZ-NH2	8.87	129.15	119.40
1	P	33	ASP	CB-CG-OD2	8.87	126.28	118.30
1	Q	303	ARG	CD-NE-CZ	8.87	136.01	123.60
1	K	152	ARG	CA-CB-CG	8.86	132.90	113.40
1	C	3	ARG	CA-C-O	-8.85	101.51	120.10
1	B	25	ASN	O-C-N	8.85	138.24	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	HIS	CB-CA-C	-8.85	92.70	110.40
1	D	87	ASP	N-CA-CB	-8.85	94.68	110.60
1	I	67	SER	O-C-N	8.84	136.84	122.70
1	R	330	ARG	NH1-CZ-NH2	-8.84	109.68	119.40
1	R	344	HIS	N-CA-CB	8.84	126.50	110.60
1	J	160	SER	O-C-N	8.83	136.83	122.70
1	D	3	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	L	330	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	G	186	VAL	CA-CB-CG2	-8.81	97.68	110.90
1	K	115	LEU	CB-CG-CD2	-8.81	96.02	111.00
1	K	191	ILE	CA-CB-CG2	8.81	128.52	110.90
1	G	152	ARG	CB-CA-C	-8.81	92.79	110.40
1	F	109	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	O	78	LEU	O-C-N	8.80	136.78	122.70
1	B	1	ALA	O-C-N	-8.80	108.62	122.70
1	B	11	GLN	CG-CD-OE1	8.80	139.20	121.60
1	F	329	LYS	CG-CD-CE	8.79	138.27	111.90
1	A	189	GLU	OE1-CD-OE2	-8.78	112.76	123.30
1	P	56	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	Q	203	TYR	CB-CG-CD1	-8.78	115.73	121.00
1	A	357	PHE	CB-CG-CD2	8.77	126.94	120.80
1	H	70	ASN	N-CA-CB	-8.77	94.81	110.60
1	D	195	ASP	CB-CG-OD2	8.77	126.19	118.30
1	L	55	ARG	CD-NE-CZ	-8.77	111.32	123.60
1	C	258	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	L	87	ASP	N-CA-CB	-8.77	94.82	110.60
1	N	94	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	F	23	VAL	CG1-CB-CG2	-8.74	96.91	110.90
1	I	195	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	G	147	TRP	O-C-N	8.74	136.68	122.70
1	O	296	LYS	CD-CE-NZ	8.74	131.79	111.70
1	N	33	ASP	CB-CG-OD2	8.73	126.16	118.30
1	G	231	ASN	O-C-N	8.73	136.67	122.70
1	F	68	SER	N-CA-CB	-8.73	97.41	110.50
1	E	148	ARG	C-N-CA	8.72	143.50	121.70
1	D	172	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	212	VAL	CA-CB-CG1	-8.69	97.87	110.90
1	D	213	TYR	CB-CG-CD2	-8.68	115.79	121.00
1	Q	226	THR	N-CA-CB	-8.68	93.80	110.30
1	A	153	ILE	O-C-N	-8.67	108.83	122.70
1	D	303	ARG	CA-C-O	-8.67	101.90	120.10
1	M	69	ILE	CG1-CB-CG2	-8.66	92.34	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	94	ARG	NE-CZ-NH1	-8.65	115.97	120.30
1	M	89	GLN	CB-CG-CD	-8.64	89.13	111.60
1	B	172	ARG	NE-CZ-NH2	8.62	124.61	120.30
1	M	1	ALA	N-CA-CB	-8.62	98.03	110.10
1	A	42	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	G	258	ARG	CB-CG-CD	8.61	133.98	111.60
1	P	2	HIS	CA-CB-CG	8.60	128.22	113.60
1	J	223	LEU	O-C-N	8.59	136.45	122.70
1	A	221	VAL	CA-CB-CG2	-8.59	98.02	110.90
1	E	346	GLY	C-N-CA	8.57	143.12	121.70
1	F	8	THR	CA-CB-CG2	-8.55	100.43	112.40
1	J	1	ALA	N-CA-CB	-8.54	98.14	110.10
1	C	42	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	L	143	ASP	CB-CG-OD1	-8.54	110.61	118.30
1	M	203	TYR	CB-CG-CD1	-8.54	115.88	121.00
1	G	243	TYR	CB-CG-CD2	-8.53	115.88	121.00
1	I	118	THR	N-CA-CB	-8.52	94.10	110.30
1	P	24	ALA	CA-C-N	8.52	135.95	117.20
1	R	199	GLU	CA-CB-CG	8.52	132.15	113.40
1	H	330	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	C	94	ARG	NH1-CZ-NH2	-8.52	110.03	119.40
1	N	55	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	267	ILE	CA-CB-CG2	8.51	127.92	110.90
1	D	270	LEU	CB-CG-CD1	-8.51	96.53	111.00
1	L	342	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	R	19	ALA	CB-CA-C	-8.50	97.35	110.10
1	C	3	ARG	NH1-CZ-NH2	-8.50	110.05	119.40
1	L	262	ALA	CB-CA-C	8.50	122.85	110.10
1	C	87	ASP	OD1-CG-OD2	8.49	139.44	123.30
1	D	186	VAL	N-CA-CB	-8.49	92.83	111.50
1	K	199	GLU	CA-CB-CG	8.49	132.07	113.40
1	N	125	GLN	CG-CD-OE1	8.49	138.57	121.60
1	A	133	ARG	CD-NE-CZ	-8.48	111.73	123.60
1	I	137	TYR	CB-CG-CD1	8.47	126.08	121.00
1	M	84	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	I	226	THR	CA-CB-CG2	8.46	124.25	112.40
1	A	204	VAL	CA-CB-CG1	8.46	123.59	110.90
1	O	191	ILE	CA-CB-CG2	8.46	127.82	110.90
1	A	348	SER	CA-C-N	8.45	133.10	116.20
1	K	88	SER	O-C-N	-8.45	109.18	122.70
1	C	24	ALA	C-N-CA	-8.44	100.59	121.70
1	K	243	TYR	CB-CG-CD1	-8.44	115.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	8	THR	OG1-CB-CG2	-8.43	90.61	110.00
1	O	262	ALA	CB-CA-C	8.43	122.75	110.10
1	F	123	THR	N-CA-CB	8.42	126.30	110.30
1	G	303	ARG	CD-NE-CZ	-8.42	111.81	123.60
1	H	195	ASP	CB-CG-OD1	-8.42	110.72	118.30
1	M	42	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	358	THR	CA-C-N	-8.41	98.70	117.20
1	B	182	LEU	O-C-N	-8.41	109.25	122.70
1	D	74	GLY	O-C-N	-8.41	108.91	123.20
1	M	60	GLU	OE1-CD-OE2	-8.41	113.21	123.30
1	E	118	THR	N-CA-CB	-8.40	94.34	110.30
1	A	24	ALA	C-N-CA	-8.40	100.71	121.70
1	I	271	SER	CA-C-O	8.39	137.73	120.10
1	B	6	ALA	CA-C-O	-8.39	102.47	120.10
1	J	248	VAL	CA-CB-CG2	-8.39	98.31	110.90
1	G	67	SER	N-CA-CB	-8.39	97.91	110.50
1	Q	258	ARG	NH1-CZ-NH2	-8.39	110.17	119.40
1	E	152	ARG	CD-NE-CZ	-8.39	111.86	123.60
1	Q	89	GLN	C-N-CA	-8.38	104.69	122.30
1	P	195	ASP	CA-CB-CG	8.38	131.84	113.40
1	N	125	GLN	OE1-CD-NE2	-8.38	102.63	121.90
1	K	25	ASN	N-CA-CB	8.38	125.68	110.60
1	Q	56	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	C	55	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	A	94	ARG	CD-NE-CZ	8.34	135.28	123.60
1	A	42	ARG	NH1-CZ-NH2	-8.34	110.22	119.40
1	C	94	ARG	CB-CG-CD	8.33	133.27	111.60
1	R	132	GLU	CG-CD-OE1	8.33	134.97	118.30
1	B	252	THR	CA-CB-CG2	-8.33	100.74	112.40
1	I	133	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	P	49	GLU	CA-CB-CG	8.33	131.72	113.40
1	P	213	TYR	CB-CG-CD1	-8.32	116.00	121.00
1	I	59	ARG	CG-CD-NE	8.32	129.27	111.80
1	D	20	GLN	CA-CB-CG	-8.32	95.10	113.40
1	B	148	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	G	276	GLU	OE1-CD-OE2	-8.31	113.32	123.30
1	J	24	ALA	N-CA-CB	8.31	121.74	110.10
1	I	195	ASP	CA-CB-CG	-8.31	95.11	113.40
1	K	248	VAL	CA-CB-CG2	-8.31	98.43	110.90
1	O	199	GLU	CA-CB-CG	8.31	131.68	113.40
1	B	42	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	C	109	ASP	CB-CG-OD2	-8.31	110.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	TYR	CB-CG-CD1	8.31	125.98	121.00
1	B	342	TYR	CB-CG-CD2	8.30	125.98	121.00
1	K	109	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	F	303	ARG	CG-CD-NE	8.29	129.22	111.80
1	K	128	ASP	CB-CG-OD2	8.29	125.76	118.30
1	P	342	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	A	87	ASP	N-CA-CB	-8.28	95.69	110.60
1	C	172	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	D	33	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	J	59	ARG	NH1-CZ-NH2	-8.27	110.30	119.40
1	E	295	TRP	CB-CG-CD2	8.26	137.34	126.60
1	H	66	ASP	CA-C-O	-8.26	102.75	120.10
1	H	118	THR	N-CA-CB	-8.26	94.61	110.30
1	F	165	GLU	OE1-CD-OE2	8.25	133.20	123.30
1	F	351	ALA	N-CA-CB	-8.25	98.55	110.10
1	N	42	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	O	330	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	O	82	THR	O-C-N	-8.23	109.53	122.70
1	P	33	ASP	CB-CG-OD1	-8.22	110.90	118.30
1	B	94	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	C	133	ARG	NH1-CZ-NH2	-8.22	110.36	119.40
1	I	191	ILE	CA-CB-CG1	-8.21	95.39	111.00
1	I	98	LYS	CD-CE-NZ	8.20	130.56	111.70
1	B	142	VAL	CA-CB-CG2	-8.20	98.60	110.90
1	F	243	TYR	CB-CG-CD1	8.20	125.92	121.00
1	O	133	ARG	CD-NE-CZ	-8.20	112.13	123.60
1	E	2	HIS	N-CA-C	8.19	133.12	111.00
1	G	109	ASP	CB-CG-OD1	-8.19	110.93	118.30
1	K	137	TYR	CB-CG-CD1	-8.18	116.09	121.00
1	R	133	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	M	345	THR	N-CA-C	8.18	133.07	111.00
1	P	87	ASP	N-CA-CB	-8.17	95.89	110.60
1	B	232	MET	CG-SD-CE	-8.17	87.13	100.20
1	K	94	ARG	CD-NE-CZ	8.16	135.03	123.60
1	K	191	ILE	CA-CB-CG1	-8.16	95.49	111.00
1	K	258	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	Q	267	ILE	CB-CA-C	8.16	127.93	111.60
1	F	110	GLN	CB-CG-CD	8.16	132.82	111.60
1	R	27	LYS	CD-CE-NZ	8.16	130.47	111.70
1	M	70	ASN	CA-CB-CG	-8.15	95.48	113.40
1	B	207	LYS	N-CA-CB	-8.14	95.94	110.60
1	J	51	THR	N-CA-CB	-8.13	94.85	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	42	ARG	NE-CZ-NH2	8.13	124.36	120.30
1	D	94	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	F	118	THR	N-CA-CB	-8.12	94.86	110.30
1	Q	258	ARG	CD-NE-CZ	8.12	134.98	123.60
1	B	55	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	E	84	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	D	321	GLU	OE1-CD-OE2	8.12	133.04	123.30
1	J	191	ILE	CA-CB-CG1	-8.12	95.58	111.00
1	K	87	ASP	OD1-CG-OD2	-8.12	107.88	123.30
1	K	172	ARG	CD-NE-CZ	-8.12	112.24	123.60
1	B	183	VAL	CB-CA-C	-8.11	95.99	111.40
1	J	197	ASP	CB-CG-OD1	8.11	125.60	118.30
1	B	71	GLN	C-N-CA	8.11	141.97	121.70
1	G	310	LEU	CA-CB-CG	8.11	133.94	115.30
1	B	303	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	E	59	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	J	68	SER	CB-CA-C	-8.09	94.73	110.10
1	B	277	GLU	OE1-CD-OE2	-8.08	113.61	123.30
1	P	328	MET	CA-CB-CG	8.08	127.03	113.30
1	M	177	CYS	CA-CB-SG	8.08	128.54	114.00
1	F	219	HIS	O-C-N	-8.07	109.78	122.70
1	Q	42	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	J	226	THR	CA-CB-CG2	8.07	123.69	112.40
1	E	195	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	Q	3	ARG	CA-C-N	8.06	134.93	117.20
1	N	118	THR	N-CA-CB	-8.04	95.02	110.30
1	O	24	ALA	CA-C-O	-8.04	103.21	120.10
1	A	118	THR	N-CA-CB	-8.04	95.03	110.30
1	G	87	ASP	CB-CA-C	-8.03	94.33	110.40
1	L	25	ASN	CA-CB-CG	8.03	131.07	113.40
1	A	87	ASP	OD1-CG-OD2	8.02	138.54	123.30
1	D	185	ILE	CA-C-N	8.02	134.84	117.20
1	D	172	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	M	33	ASP	CB-CG-OD1	8.02	125.52	118.30
1	N	133	ARG	CD-NE-CZ	-8.01	112.38	123.60
1	I	87	ASP	OD1-CG-OD2	8.01	138.51	123.30
1	J	25	ASN	CA-CB-CG	8.01	131.02	113.40
1	P	152	ARG	NH1-CZ-NH2	8.00	128.20	119.40
1	L	197	ASP	CB-CG-OD1	7.99	125.49	118.30
1	D	303	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	C	213	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	I	222	TYR	CB-CG-CD1	-7.97	116.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	226	THR	CA-C-N	7.97	134.73	117.20
1	F	244	THR	N-CA-CB	-7.97	95.16	110.30
1	I	89	GLN	N-CA-CB	-7.97	96.26	110.60
1	F	344	HIS	N-CA-CB	7.96	124.93	110.60
1	M	258	ARG	CD-NE-CZ	7.96	134.74	123.60
1	P	173	TYR	CB-CG-CD2	-7.96	116.23	121.00
1	B	7	LEU	CB-CG-CD1	7.95	124.52	111.00
1	N	186	VAL	O-C-N	-7.95	109.98	122.70
1	J	203	TYR	CB-CG-CD2	7.95	125.77	121.00
1	I	203	TYR	CB-CG-CD2	7.95	125.77	121.00
1	P	1	ALA	CB-CA-C	7.94	122.01	110.10
1	L	128	ASP	CB-CG-OD1	-7.94	111.16	118.30
1	I	148	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	P	278	ASP	CB-CG-OD2	7.93	125.44	118.30
1	D	89	GLN	N-CA-CB	-7.93	96.33	110.60
1	F	124	ILE	CG1-CB-CG2	-7.93	93.96	111.40
1	B	87	ASP	CA-C-O	-7.92	103.46	120.10
1	F	214	LYS	CD-CE-NZ	-7.92	93.49	111.70
1	C	25	ASN	O-C-N	7.92	136.66	123.20
1	A	345	THR	N-CA-C	-7.91	89.65	111.00
1	R	309	ALA	CB-CA-C	-7.90	98.25	110.10
1	J	45	ARG	NH1-CZ-NH2	7.90	128.09	119.40
1	B	243	TYR	CB-CG-CD1	7.89	125.73	121.00
1	D	325	GLU	CB-CG-CD	-7.89	92.89	114.20
1	I	66	ASP	CA-C-O	7.89	136.67	120.10
1	H	94	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	193	ASP	CB-CG-OD1	7.88	125.39	118.30
1	H	2	HIS	CA-C-N	7.88	134.53	117.20
1	I	24	ALA	CB-CA-C	-7.87	98.29	110.10
1	B	23	VAL	CG1-CB-CG2	-7.87	98.31	110.90
1	C	342	TYR	CB-CG-CD1	-7.87	116.28	121.00
1	H	190	VAL	CA-CB-CG2	7.87	122.71	110.90
1	D	195	ASP	CA-CB-CG	7.87	130.71	113.40
1	D	327	PHE	CG-CD1-CE1	7.87	129.46	120.80
1	N	243	TYR	CB-CG-CD1	7.87	125.72	121.00
1	O	328	MET	CB-CA-C	7.87	126.13	110.40
1	R	171	ALA	N-CA-CB	7.86	121.11	110.10
1	M	278	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	94	ARG	NH1-CZ-NH2	-7.86	110.76	119.40
1	E	148	ARG	O-C-N	-7.85	110.14	122.70
1	K	161	LEU	CB-CG-CD1	7.84	124.33	111.00
1	J	199	GLU	OE1-CD-OE2	-7.83	113.90	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	LEU	N-CA-CB	7.83	126.06	110.40
1	D	214	LYS	N-CA-CB	-7.83	96.51	110.60
1	R	121	GLU	CA-C-O	7.83	136.53	120.10
1	A	14	GLU	OE1-CD-OE2	-7.82	113.91	123.30
1	A	164	GLN	CA-CB-CG	7.82	130.61	113.40
1	I	67	SER	CA-CB-OG	-7.82	90.10	111.20
1	N	1	ALA	CA-C-O	-7.81	103.70	120.10
1	H	344	HIS	CA-C-O	7.81	136.49	120.10
1	G	323	THR	CA-CB-CG2	-7.80	101.48	112.40
1	M	24	ALA	CA-C-O	-7.80	103.73	120.10
1	F	344	HIS	C-N-CA	7.79	141.18	121.70
1	C	226	THR	N-CA-CB	-7.79	95.50	110.30
1	C	195	ASP	N-CA-CB	-7.79	96.59	110.60
1	Q	51	THR	N-CA-CB	-7.78	95.52	110.30
1	A	33	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	A	237	HIS	CA-CB-CG	-7.77	100.39	113.60
1	F	330	ARG	CG-CD-NE	7.77	128.11	111.80
1	O	84	TYR	CB-CG-CD2	-7.77	116.34	121.00
1	E	221	VAL	CA-CB-CG2	-7.76	99.25	110.90
1	F	352	SER	CA-C-O	7.76	136.40	120.10
1	B	11	GLN	CA-C-N	-7.76	100.13	117.20
1	N	59	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	L	25	ASN	O-C-N	7.75	136.37	123.20
1	Q	291	LEU	CA-CB-CG	7.75	133.12	115.30
1	H	84	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	Q	42	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	H	171	ALA	CA-C-O	-7.74	103.85	120.10
1	Q	199	GLU	CB-CG-CD	7.74	135.09	114.20
1	D	87	ASP	CA-CB-CG	-7.74	96.38	113.40
1	P	243	TYR	C-N-CA	7.73	141.02	121.70
1	P	109	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	K	258	ARG	CA-CB-CG	7.72	130.39	113.40
1	A	248	VAL	CA-CB-CG2	-7.72	99.32	110.90
1	P	218	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	O	3	ARG	CD-NE-CZ	7.72	134.40	123.60
1	H	89	GLN	CB-CG-CD	-7.71	91.55	111.60
1	C	344	HIS	CA-CB-CG	-7.71	100.49	113.60
1	P	152	ARG	CD-NE-CZ	-7.71	112.81	123.60
1	D	185	ILE	O-C-N	-7.71	110.37	122.70
1	H	237	HIS	CB-CA-C	-7.71	94.99	110.40
1	I	115	LEU	O-C-N	-7.70	110.38	122.70
1	Q	59	ARG	CD-NE-CZ	7.69	134.37	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	128	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	B	5	PRO	CA-C-N	-7.68	100.31	117.20
1	D	348	SER	C-N-CA	7.68	138.42	122.30
1	N	260	VAL	CG1-CB-CG2	7.68	123.18	110.90
1	D	155	ASP	CB-CG-OD1	-7.67	111.39	118.30
1	H	4	PHE	CB-CG-CD2	-7.67	115.43	120.80
1	R	177	CYS	CA-CB-SG	7.67	127.80	114.00
1	F	250	MET	CG-SD-CE	-7.67	87.93	100.20
1	H	8	THR	CA-CB-CG2	7.67	123.13	112.40
1	L	42	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	R	293	LYS	CB-CG-CD	-7.67	91.67	111.60
1	B	300	SER	N-CA-CB	7.66	121.99	110.50
1	H	234	THR	CA-CB-CG2	7.66	123.13	112.40
1	R	343	VAL	CA-C-O	-7.66	104.02	120.10
1	I	25	ASN	O-C-N	7.65	136.21	123.20
1	R	8	THR	CA-CB-CG2	-7.65	101.68	112.40
1	H	96	ILE	O-C-N	7.65	134.94	122.70
1	D	301	TYR	O-C-N	-7.65	110.20	123.20
1	O	3	ARG	CA-CB-CG	7.64	130.21	113.40
1	P	325	GLU	OE1-CD-OE2	7.64	132.47	123.30
1	O	3	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	N	4	PHE	CB-CG-CD1	7.63	126.14	120.80
1	D	327	PHE	CB-CG-CD2	7.63	126.14	120.80
1	N	284	ASN	OD1-CG-ND2	-7.63	104.36	121.90
1	I	82	THR	CA-CB-CG2	-7.62	101.73	112.40
1	B	281	LEU	CB-CG-CD1	-7.62	98.04	111.00
1	Q	301	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	B	33	ASP	CB-CG-OD1	7.62	125.16	118.30
1	O	210	ALA	CB-CA-C	7.62	121.53	110.10
1	B	121	GLU	OE1-CD-OE2	7.61	132.43	123.30
1	D	152	ARG	CD-NE-CZ	-7.60	112.96	123.60
1	L	218	ASP	CB-CG-OD2	-7.59	111.46	118.30
1	D	268	CYS	N-CA-CB	-7.59	96.94	110.60
1	I	137	TYR	CB-CG-CD2	-7.59	116.45	121.00
1	M	69	ILE	C-N-CA	7.59	140.68	121.70
1	O	24	ALA	N-CA-CB	7.59	120.73	110.10
1	D	221	VAL	CA-CB-CG2	-7.59	99.52	110.90
1	J	344	HIS	C-N-CA	7.58	140.65	121.70
1	Q	109	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	J	94	ARG	CA-CB-CG	7.58	130.07	113.40
1	M	161	LEU	CB-CG-CD2	-7.58	98.12	111.00
1	Q	87	ASP	N-CA-CB	-7.58	96.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	ASP	CB-CG-OD2	7.57	125.11	118.30
1	J	339	LYS	CA-CB-CG	7.57	130.06	113.40
1	R	89	GLN	N-CA-CB	-7.57	96.97	110.60
1	A	148	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	E	84	TYR	CB-CG-CD1	7.56	125.54	121.00
1	F	110	GLN	CG-CD-NE2	-7.56	98.55	116.70
1	L	55	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	E	207	LYS	CD-CE-NZ	7.55	129.07	111.70
1	I	133	ARG	C-N-CA	-7.55	102.82	121.70
1	O	45	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	D	42	ARG	CD-NE-CZ	7.55	134.17	123.60
1	K	42	ARG	CD-NE-CZ	7.54	134.16	123.60
1	O	258	ARG	NH1-CZ-NH2	7.54	127.69	119.40
1	L	342	TYR	CB-CG-CD1	7.53	125.52	121.00
1	H	1	ALA	N-CA-C	7.53	131.33	111.00
1	A	118	THR	OG1-CB-CG2	7.53	127.31	110.00
1	A	99	GLU	OE1-CD-OE2	7.53	132.33	123.30
1	L	2	HIS	N-CA-CB	7.53	124.15	110.60
1	L	303	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	J	123	THR	N-CA-CB	7.52	124.58	110.30
1	R	24	ALA	CB-CA-C	-7.51	98.83	110.10
1	A	258	ARG	CA-CB-CG	7.51	129.91	113.40
1	I	69	ILE	C-N-CA	7.50	140.46	121.70
1	D	66	ASP	CA-CB-CG	7.50	129.91	113.40
1	G	152	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	L	143	ASP	OD1-CG-OD2	7.50	137.56	123.30
1	B	104	VAL	CB-CA-C	-7.49	97.16	111.40
1	G	172	ARG	CD-NE-CZ	7.49	134.09	123.60
1	E	109	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	F	56	ARG	CD-NE-CZ	7.48	134.08	123.60
1	K	140	ASP	CB-CG-OD1	-7.48	111.56	118.30
1	C	328	MET	N-CA-CB	-7.48	97.14	110.60
1	G	24	ALA	C-N-CA	-7.48	103.00	121.70
1	B	212	VAL	N-CA-CB	-7.48	95.05	111.50
1	G	172	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	F	352	SER	O-C-N	-7.47	110.74	122.70
1	D	21	SER	O-C-N	7.47	134.65	122.70
1	H	203	TYR	CB-CG-CD2	7.47	125.48	121.00
1	Q	59	ARG	CG-CD-NE	7.47	127.48	111.80
1	H	207	LYS	CD-CE-NZ	7.46	128.87	111.70
1	B	269	PHE	CB-CG-CD1	7.46	126.02	120.80
1	G	59	ARG	NE-CZ-NH2	7.45	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	123	THR	N-CA-CB	7.45	124.45	110.30
1	H	244	THR	OG1-CB-CG2	-7.44	92.88	110.00
1	B	160	SER	CB-CA-C	-7.44	95.97	110.10
1	G	8	THR	CA-CB-CG2	-7.43	101.99	112.40
1	G	66	ASP	O-C-N	7.43	134.59	122.70
1	F	116	ALA	C-N-CA	7.43	137.90	122.30
1	A	303	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	E	24	ALA	N-CA-CB	7.42	120.49	110.10
1	F	267	ILE	CG1-CB-CG2	-7.42	95.07	111.40
1	B	255	ALA	N-CA-CB	-7.42	99.71	110.10
1	D	51	THR	CA-CB-CG2	7.42	122.78	112.40
1	J	352	SER	CA-C-O	7.42	135.67	120.10
1	E	143	ASP	CB-CG-OD1	7.41	124.97	118.30
1	Q	203	TYR	CB-CG-CD2	7.41	125.44	121.00
1	B	258	ARG	CD-NE-CZ	7.40	133.97	123.60
1	J	246	GLU	OE1-CD-OE2	-7.40	114.42	123.30
1	C	87	ASP	N-CA-CB	-7.40	97.28	110.60
1	O	168	ASN	N-CA-CB	7.40	123.92	110.60
1	Q	81	GLU	OE1-CD-OE2	-7.40	114.42	123.30
1	I	59	ARG	CD-NE-CZ	-7.39	113.25	123.60
1	N	56	ARG	CD-NE-CZ	-7.39	113.25	123.60
1	P	356	LEU	CA-C-N	7.39	133.47	117.20
1	D	148	ARG	NH1-CZ-NH2	7.38	127.52	119.40
1	F	128	ASP	OD1-CG-OD2	7.38	137.33	123.30
1	L	87	ASP	CB-CG-OD1	-7.38	111.66	118.30
1	B	6	ALA	CB-CA-C	-7.37	99.04	110.10
1	D	152	ARG	CB-CA-C	-7.37	95.65	110.40
1	F	25	ASN	CA-CB-CG	7.37	129.60	113.40
1	E	349	GLY	N-CA-C	-7.36	94.69	113.10
1	A	278	ASP	CB-CG-OD2	7.35	124.92	118.30
1	I	87	ASP	N-CA-CB	7.35	123.83	110.60
1	O	98	LYS	CD-CE-NZ	7.35	128.61	111.70
1	A	149	ALA	CB-CA-C	-7.35	99.08	110.10
1	I	143	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	Q	89	GLN	CB-CA-C	-7.35	95.71	110.40
1	D	190	VAL	C-N-CA	7.34	140.06	121.70
1	F	89	GLN	CB-CG-CD	-7.34	92.51	111.60
1	M	3	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	Q	267	ILE	CA-CB-CG1	-7.34	97.05	111.00
1	H	132	GLU	OE1-CD-OE2	-7.34	114.50	123.30
1	N	109	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	B	211	ALA	CA-C-N	-7.33	101.07	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	347	SER	CA-C-N	-7.33	101.07	117.20
1	P	353	THR	CA-CB-CG2	-7.33	102.14	112.40
1	L	38	THR	CA-CB-CG2	-7.33	102.14	112.40
1	K	357	PHE	N-CA-CB	7.32	123.77	110.60
1	B	33	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	N	81	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	Q	10	GLU	CB-CA-C	-7.31	95.78	110.40
1	C	152	ARG	CD-NE-CZ	-7.31	113.37	123.60
1	C	186	VAL	O-C-N	-7.30	111.01	122.70
1	E	299	PHE	O-C-N	-7.30	111.01	122.70
1	F	231	ASN	CB-CA-C	-7.30	95.79	110.40
1	J	342	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	L	204	VAL	CA-CB-CG2	-7.30	99.95	110.90
1	I	342	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	P	357	PHE	CB-CG-CD1	7.30	125.91	120.80
1	L	113	ALA	N-CA-CB	7.30	120.31	110.10
1	N	221	VAL	CA-CB-CG1	-7.30	99.95	110.90
1	R	123	THR	CA-CB-OG1	7.30	124.32	109.00
1	R	141	GLY	CA-C-O	-7.29	107.47	120.60
1	C	32	ALA	N-CA-CB	-7.29	99.89	110.10
1	P	221	VAL	CA-CB-CG2	-7.29	99.96	110.90
1	H	344	HIS	CB-CA-C	-7.29	95.82	110.40
1	H	267	ILE	CA-CB-CG2	7.28	125.45	110.90
1	Q	165	GLU	CG-CD-OE2	-7.28	103.75	118.30
1	H	133	ARG	CD-NE-CZ	7.27	133.78	123.60
1	E	295	TRP	O-C-N	7.27	134.33	122.70
1	G	195	ASP	N-CA-CB	-7.27	97.52	110.60
1	D	154	ALA	CB-CA-C	-7.26	99.21	110.10
1	H	218	ASP	CB-CG-OD1	7.26	124.83	118.30
1	R	51	THR	N-CA-CB	-7.26	96.51	110.30
1	F	190	VAL	C-N-CA	7.26	139.84	121.70
1	L	226	THR	N-CA-CB	-7.26	96.51	110.30
1	M	137	TYR	O-C-N	-7.25	111.10	122.70
1	A	243	TYR	C-N-CA	7.25	139.81	121.70
1	K	258	ARG	N-CA-CB	7.23	123.61	110.60
1	H	173	TYR	CB-CG-CD1	7.23	125.34	121.00
1	P	138	LYS	O-C-N	7.23	134.26	122.70
1	E	249	ALA	CB-CA-C	7.22	120.93	110.10
1	P	222	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	K	133	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	N	156	GLN	CA-CB-CG	-7.22	97.52	113.40
1	P	297	LEU	CB-CG-CD2	-7.21	98.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	HIS	CA-CB-CG	-7.21	101.34	113.60
1	Q	42	ARG	NH1-CZ-NH2	-7.21	111.47	119.40
1	O	89	GLN	CA-C-N	7.21	130.62	116.20
1	I	81	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	E	71	GLN	C-N-CA	7.21	139.72	121.70
1	B	93	PHE	CE1-CZ-CE2	-7.20	107.03	120.00
1	H	353	THR	CA-C-O	7.20	135.22	120.10
1	A	217	ASN	CB-CG-OD1	7.20	136.00	121.60
1	B	27	LYS	CG-CD-CE	-7.20	90.30	111.90
1	I	67	SER	C-N-CA	-7.20	103.71	121.70
1	D	151	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	F	51	THR	N-CA-CB	-7.20	96.63	110.30
1	H	56	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	357	PHE	N-CA-C	7.19	130.43	111.00
1	I	88	SER	N-CA-CB	7.19	121.29	110.50
1	L	143	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	279	ALA	N-CA-CB	7.19	120.17	110.10
1	G	81	GLU	OE1-CD-OE2	-7.19	114.68	123.30
1	J	2	HIS	CA-C-N	7.18	133.01	117.20
1	L	191	ILE	CG1-CB-CG2	-7.18	95.59	111.40
1	I	165	GLU	CB-CA-C	7.18	124.75	110.40
1	E	42	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	D	152	ARG	CB-CG-CD	7.17	130.25	111.60
1	K	265	PRO	C-N-CA	-7.17	107.24	122.30
1	E	155	ASP	CB-CG-OD2	7.17	124.75	118.30
1	P	65	VAL	CA-CB-CG2	7.17	121.66	110.90
1	J	92	LEU	O-C-N	-7.17	111.23	122.70
1	K	299	PHE	CG-CD2-CE2	7.17	128.68	120.80
1	P	45	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	241	LYS	N-CA-CB	7.17	123.50	110.60
1	M	24	ALA	C-N-CA	-7.17	103.79	121.70
1	J	99	GLU	OE1-CD-OE2	7.16	131.90	123.30
1	J	166	ASN	CB-CG-ND2	7.16	133.89	116.70
1	R	214	LYS	CD-CE-NZ	-7.16	95.23	111.70
1	C	3	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	E	132	GLU	CB-CG-CD	7.16	133.52	114.20
1	J	130	LEU	CB-CG-CD2	-7.15	98.84	111.00
1	E	165	GLU	CG-CD-OE2	-7.15	104.00	118.30
1	F	89	GLN	CB-CA-C	-7.15	96.10	110.40
1	Q	210	ALA	CB-CA-C	-7.15	99.37	110.10
1	C	38	THR	CA-CB-CG2	-7.15	102.39	112.40
1	C	111	GLY	CA-C-O	7.14	133.45	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	TYR	CB-CG-CD1	-7.14	116.72	121.00
1	B	207	LYS	CG-CD-CE	7.14	133.31	111.90
1	F	348	SER	CA-C-O	7.13	135.08	120.10
1	M	227	LEU	CB-CG-CD1	-7.13	98.87	111.00
1	B	21	SER	O-C-N	7.13	134.10	122.70
1	B	300	SER	N-CA-C	-7.13	91.76	111.00
1	P	253	VAL	CG1-CB-CG2	-7.13	99.50	110.90
1	I	173	TYR	CB-CG-CD2	-7.12	116.72	121.00
1	I	36	VAL	CA-CB-CG1	-7.12	100.22	110.90
1	Q	133	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	R	224	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	G	20	GLN	O-C-N	-7.12	111.31	122.70
1	P	179	GLN	CG-CD-OE1	-7.12	107.36	121.60
1	D	68	SER	CB-CA-C	-7.11	96.59	110.10
1	F	70	ASN	N-CA-CB	-7.11	97.79	110.60
1	O	97	LEU	CB-CG-CD1	-7.11	98.91	111.00
1	P	213	TYR	CZ-CE2-CD2	-7.11	113.40	119.80
1	O	182	LEU	CB-CG-CD2	-7.11	98.91	111.00
1	D	3	ARG	CA-CB-CG	7.11	129.04	113.40
1	E	152	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	I	70	ASN	O-C-N	7.10	134.06	122.70
1	B	24	ALA	N-CA-CB	7.10	120.04	110.10
1	E	256	LEU	CA-C-O	7.10	135.00	120.10
1	A	55	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	J	195	ASP	CB-CA-C	-7.10	96.21	110.40
1	D	207	LYS	CA-CB-CG	7.09	129.00	113.40
1	E	348	SER	CA-C-N	-7.09	102.02	116.20
1	R	132	GLU	OE1-CD-OE2	-7.09	114.79	123.30
1	D	188	PRO	O-C-N	7.09	134.04	122.70
1	J	113	ALA	O-C-N	7.08	134.55	121.10
1	C	36	VAL	CA-CB-CG1	-7.08	100.28	110.90
1	L	322	ALA	CB-CA-C	-7.08	99.48	110.10
1	H	344	HIS	CA-C-N	-7.08	101.63	117.20
1	O	195	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	228	LEU	CA-CB-CG	7.07	131.56	115.30
1	F	127	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	B	267	ILE	CB-CG1-CD1	-7.05	94.15	113.90
1	P	342	TYR	CB-CG-CD1	7.05	125.23	121.00
1	I	68	SER	CA-C-O	-7.04	105.31	120.10
1	J	352	SER	N-CA-CB	7.04	121.06	110.50
1	K	68	SER	CB-CA-C	-7.04	96.72	110.10
1	M	224	GLU	CA-CB-CG	7.04	128.89	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	226	THR	N-CA-CB	-7.04	96.93	110.30
1	F	152	ARG	NH1-CZ-NH2	7.04	127.14	119.40
1	R	203	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	C	118	THR	N-CA-CB	-7.03	96.94	110.30
1	H	66	ASP	CB-CG-OD1	7.03	124.63	118.30
1	P	94	ARG	CD-NE-CZ	7.03	133.44	123.60
1	L	80	HIS	CB-CA-C	-7.02	96.35	110.40
1	C	132	GLU	CG-CD-OE1	7.02	132.34	118.30
1	L	252	THR	CA-CB-CG2	-7.02	102.57	112.40
1	B	79	PHE	CB-CG-CD1	-7.02	115.89	120.80
1	M	199	GLU	CB-CA-C	7.02	124.44	110.40
1	K	53	GLU	OE1-CD-OE2	7.02	131.72	123.30
1	I	329	LYS	CA-CB-CG	7.01	128.82	113.40
1	P	277	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	A	207	LYS	CG-CD-CE	7.01	132.93	111.90
1	D	193	ASP	CB-CG-OD2	-7.01	112.00	118.30
1	E	267	ILE	CA-CB-CG2	7.01	124.91	110.90
1	J	42	ARG	CD-NE-CZ	7.01	133.41	123.60
1	R	102	ILE	CA-CB-CG1	-7.01	97.69	111.00
1	E	256	LEU	O-C-N	-7.00	111.50	122.70
1	P	343	VAL	CB-CA-C	-7.00	98.10	111.40
1	J	161	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	O	118	THR	N-CA-CB	-7.00	97.00	110.30
1	Q	60	GLU	OE1-CD-OE2	-7.00	114.91	123.30
1	B	233	VAL	CG1-CB-CG2	-6.99	99.71	110.90
1	H	132	GLU	CG-CD-OE1	6.99	132.29	118.30
1	D	216	LEU	CB-CA-C	-6.99	96.92	110.20
1	R	67	SER	O-C-N	-6.99	111.52	122.70
1	I	258	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	N	336	GLN	CA-CB-CG	6.99	128.77	113.40
1	H	186	VAL	O-C-N	-6.98	111.53	122.70
1	J	154	ALA	CB-CA-C	-6.98	99.63	110.10
1	A	165	GLU	N-CA-CB	-6.98	98.04	110.60
1	H	199	GLU	O-C-N	-6.97	111.54	122.70
1	A	196	HIS	N-CA-CB	-6.97	98.05	110.60
1	L	152	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	N	173	TYR	CB-CG-CD1	6.97	125.18	121.00
1	L	195	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	G	155	ASP	CB-CG-OD1	6.96	124.57	118.30
1	K	353	THR	CA-CB-CG2	6.96	122.15	112.40
1	G	328	MET	CG-SD-CE	6.96	111.34	100.20
1	D	344	HIS	C-N-CA	6.96	139.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	301	TYR	CB-CG-CD2	6.96	125.17	121.00
1	C	4	PHE	CB-CG-CD2	-6.96	115.93	120.80
1	G	218	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	G	267	ILE	CB-CA-C	6.95	125.51	111.60
1	I	115	LEU	CB-CA-C	6.95	123.41	110.20
1	P	248	VAL	CA-C-N	-6.95	101.91	117.20
1	L	24	ALA	CB-CA-C	-6.95	99.67	110.10
1	E	352	SER	CA-C-N	-6.95	101.91	117.20
1	C	27	LYS	CG-CD-CE	6.95	132.74	111.90
1	Q	186	VAL	CA-CB-CG2	-6.95	100.48	110.90
1	K	51	THR	N-CA-CB	-6.94	97.11	110.30
1	N	260	VAL	CA-CB-CG1	-6.94	100.50	110.90
1	B	267	ILE	C-N-CA	6.94	139.04	121.70
1	O	91	LYS	CA-CB-CG	-6.94	98.14	113.40
1	E	75	GLY	O-C-N	6.93	133.80	122.70
1	G	203	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	R	30	LEU	CB-CA-C	-6.93	97.03	110.20
1	C	258	ARG	CG-CD-NE	-6.92	97.26	111.80
1	M	344	HIS	N-CA-C	-6.92	92.30	111.00
1	B	56	ARG	CD-NE-CZ	-6.92	113.91	123.60
1	O	71	GLN	C-N-CA	6.92	139.00	121.70
1	B	90	GLY	CA-C-N	6.91	132.41	117.20
1	L	10	GLU	CB-CA-C	-6.91	96.58	110.40
1	A	183	VAL	CA-CB-CG2	-6.91	100.54	110.90
1	O	248	VAL	CA-CB-CG2	-6.91	100.54	110.90
1	L	45	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	I	11	GLN	CG-CD-OE1	6.90	135.41	121.60
1	M	11	GLN	CG-CD-OE1	6.90	135.41	121.60
1	C	249	ALA	CB-CA-C	6.90	120.45	110.10
1	C	43	LEU	CB-CG-CD2	-6.89	99.28	111.00
1	F	173	TYR	CB-CG-CD2	6.89	125.14	121.00
1	B	227	LEU	N-CA-CB	-6.89	96.61	110.40
1	E	89	GLN	C-N-CA	6.89	136.78	122.30
1	A	157	CYS	N-CA-CB	-6.89	98.20	110.60
1	D	137	TYR	CB-CG-CD1	6.89	125.13	121.00
1	D	187	GLU	CG-CD-OE1	-6.89	104.53	118.30
1	C	2	HIS	CB-CA-C	-6.88	96.63	110.40
1	O	89	GLN	CB-CG-CD	-6.88	93.70	111.60
1	J	173	TYR	CG-CD2-CE2	-6.88	115.80	121.30
1	J	277	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	P	164	GLN	CA-CB-CG	6.88	128.53	113.40
1	B	198	LEU	CB-CG-CD1	-6.87	99.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ASP	CB-CG-OD2	6.87	124.48	118.30
1	N	10	GLU	CB-CA-C	-6.87	96.65	110.40
1	N	186	VAL	CA-CB-CG1	6.87	121.21	110.90
1	N	284	ASN	CB-CG-ND2	6.87	133.19	116.70
1	B	26	GLY	C-N-CA	-6.87	104.53	121.70
1	H	1	ALA	O-C-N	-6.86	111.72	122.70
1	M	164	GLN	CA-CB-CG	6.86	128.50	113.40
1	H	1	ALA	N-CA-CB	-6.86	100.50	110.10
1	J	89	GLN	CB-CA-C	-6.86	96.68	110.40
1	A	357	PHE	C-N-CA	6.86	138.84	121.70
1	P	51	THR	N-CA-CB	-6.86	97.27	110.30
1	R	70	ASN	N-CA-CB	-6.86	98.26	110.60
1	J	137	TYR	CG-CD2-CE2	6.85	126.78	121.30
1	B	133	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	D	1	ALA	O-C-N	-6.85	111.74	122.70
1	B	18	ILE	CA-CB-CG1	-6.84	97.99	111.00
1	B	201	CYS	N-CA-CB	-6.84	98.29	110.60
1	J	10	GLU	CA-CB-CG	6.84	128.45	113.40
1	A	67	SER	CB-CA-C	-6.84	97.11	110.10
1	B	178	GLN	CA-CB-CG	-6.84	98.36	113.40
1	B	7	LEU	N-CA-CB	6.83	124.07	110.40
1	D	160	SER	C-N-CA	-6.83	104.61	121.70
1	I	260	VAL	CG1-CB-CG2	6.83	121.83	110.90
1	I	300	SER	N-CA-CB	6.83	120.75	110.50
1	D	66	ASP	CB-CG-OD1	6.83	124.45	118.30
1	E	310	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	H	82	THR	CA-CB-CG2	-6.83	102.84	112.40
1	Q	7	LEU	CA-CB-CG	6.83	131.01	115.30
1	D	152	ARG	N-CA-CB	6.83	122.89	110.60
1	M	99	GLU	OE1-CD-OE2	6.83	131.50	123.30
1	L	307	ALA	CB-CA-C	-6.83	99.86	110.10
1	N	59	ARG	CB-CG-CD	6.83	129.34	111.60
1	G	274	MET	CG-SD-CE	6.82	111.12	100.20
1	E	3	ARG	O-C-N	-6.82	111.79	122.70
1	I	68	SER	N-CA-CB	-6.82	100.28	110.50
1	R	132	GLU	N-CA-CB	6.82	122.87	110.60
1	A	243	TYR	CZ-CE2-CD2	6.81	125.93	119.80
1	J	114	PRO	C-N-CA	6.81	138.72	121.70
1	Q	151	LEU	CB-CG-CD2	-6.81	99.42	111.00
1	M	69	ILE	CA-C-N	-6.81	102.22	117.20
1	N	2	HIS	CA-CB-CG	6.81	125.17	113.60
1	J	17	GLU	OE1-CD-OE2	-6.80	115.14	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	160	SER	N-CA-CB	6.80	120.70	110.50
1	O	132	GLU	CG-CD-OE1	6.80	131.90	118.30
1	O	278	ASP	CB-CG-OD2	6.80	124.42	118.30
1	D	228	LEU	O-C-N	6.80	133.57	122.70
1	J	71	GLN	CA-CB-CG	6.79	128.34	113.40
1	A	182	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	A	343	VAL	N-CA-CB	6.79	126.44	111.50
1	E	258	ARG	CA-CB-CG	6.79	128.33	113.40
1	L	14	GLU	OE1-CD-OE2	-6.79	115.15	123.30
1	B	218	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	B	303	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	221	VAL	CA-CB-CG2	-6.78	100.73	110.90
1	K	195	ASP	OD1-CG-OD2	6.78	136.19	123.30
1	O	258	ARG	CD-NE-CZ	6.78	133.10	123.60
1	G	60	GLU	O-C-N	6.78	133.55	122.70
1	D	225	GLY	O-C-N	6.78	133.54	122.70
1	M	189	GLU	O-C-N	6.78	133.54	122.70
1	P	142	VAL	CA-CB-CG1	6.77	121.06	110.90
1	B	118	THR	N-CA-CB	-6.77	97.43	110.30
1	B	215	ALA	CB-CA-C	-6.77	99.94	110.10
1	G	71	GLN	O-C-N	6.77	133.54	122.70
1	J	209	LEU	O-C-N	6.77	133.53	122.70
1	N	64	SER	O-C-N	-6.77	111.87	122.70
1	L	148	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	C	339	LYS	N-CA-CB	6.76	122.77	110.60
1	C	107	LYS	O-C-N	-6.76	111.88	122.70
1	D	303	ARG	O-C-N	6.76	133.52	122.70
1	P	354	GLN	N-CA-C	6.76	129.25	111.00
1	A	226	THR	N-CA-CB	-6.76	97.46	110.30
1	D	51	THR	N-CA-CB	-6.75	97.47	110.30
1	L	195	ASP	N-CA-CB	-6.75	98.45	110.60
1	I	237	HIS	CA-CB-CG	-6.75	102.12	113.60
1	C	203	TYR	CB-CG-CD2	6.75	125.05	121.00
1	N	213	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	K	42	ARG	NH1-CZ-NH2	-6.75	111.98	119.40
1	K	66	ASP	OD1-CG-OD2	-6.75	110.48	123.30
1	M	165	GLU	CG-CD-OE1	6.75	131.79	118.30
1	L	300	SER	N-CA-C	-6.74	92.81	111.00
1	A	338	ALA	CB-CA-C	-6.74	100.00	110.10
1	F	155	ASP	CB-CG-OD1	6.74	124.36	118.30
1	O	301	TYR	CB-CG-CD1	-6.74	116.96	121.00
1	P	263	ALA	O-C-N	-6.74	111.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	343	VAL	CA-C-N	6.74	132.02	117.20
1	R	109	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	195	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	B	212	VAL	C-N-CA	-6.73	104.87	121.70
1	B	282	ASN	O-C-N	-6.73	111.93	122.70
1	G	232	MET	CG-SD-CE	6.73	110.97	100.20
1	R	59	ARG	NH1-CZ-NH2	6.73	126.80	119.40
1	N	316	LYS	CB-CG-CD	6.72	129.08	111.60
1	O	203	TYR	CA-CB-CG	-6.72	100.62	113.40
1	K	93	PHE	CG-CD1-CE1	6.72	128.19	120.80
1	D	224	GLU	CB-CG-CD	6.72	132.35	114.20
1	D	86	LYS	C-N-CA	6.72	138.50	121.70
1	J	24	ALA	CB-CA-C	-6.72	100.02	110.10
1	O	56	ARG	CD-NE-CZ	-6.71	114.20	123.60
1	G	103	VAL	CA-CB-CG1	-6.71	100.83	110.90
1	G	72	SER	N-CA-CB	-6.71	100.44	110.50
1	I	123	THR	CB-CA-C	-6.71	93.49	111.60
1	P	104	VAL	CG1-CB-CG2	-6.71	100.17	110.90
1	H	199	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	N	71	GLN	OE1-CD-NE2	6.70	137.31	121.90
1	A	213	TYR	CG-CD1-CE1	-6.70	115.94	121.30
1	K	9	GLN	N-CA-CB	6.70	122.65	110.60
1	J	125	GLN	CG-CD-OE1	-6.69	108.21	121.60
1	K	99	GLU	CA-C-O	-6.69	106.05	120.10
1	M	118	THR	N-CA-CB	-6.69	97.59	110.30
1	N	2	HIS	C-N-CA	6.69	138.43	121.70
1	I	67	SER	CA-C-N	-6.69	102.48	117.20
1	R	148	ARG	O-C-N	-6.69	112.00	122.70
1	L	155	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	P	199	GLU	CA-CB-CG	6.69	128.11	113.40
1	B	212	VAL	CA-CB-CG2	-6.68	100.88	110.90
1	D	70	ASN	CB-CG-ND2	-6.68	100.66	116.70
1	H	25	ASN	CA-CB-CG	6.68	128.10	113.40
1	R	147	TRP	CE3-CZ3-CH2	6.68	128.55	121.20
1	J	321	GLU	OE1-CD-OE2	6.68	131.31	123.30
1	K	195	ASP	CB-CA-C	-6.68	97.04	110.40
1	B	4	PHE	CB-CG-CD1	-6.68	116.12	120.80
1	F	278	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	220	HIS	O-C-N	6.68	133.38	122.70
1	H	13	LYS	CB-CA-C	6.68	123.75	110.40
1	L	33	ASP	CB-CG-OD1	6.68	124.31	118.30
1	M	199	GLU	OE1-CD-OE2	-6.68	115.29	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	K	165	GLU	N-CA-CB	-6.67	98.59	110.60
1	M	343	VAL	CB-CA-C	-6.67	98.72	111.40
1	N	24	ALA	C-N-CA	-6.67	105.01	121.70
1	I	3	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	R	258	ARG	NH1-CZ-NH2	-6.67	112.06	119.40
1	L	258	ARG	CG-CD-NE	-6.67	97.80	111.80
1	Q	59	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	B	174	ALA	N-CA-CB	6.66	119.43	110.10
1	E	153	ILE	CA-CB-CG2	6.66	124.22	110.90
1	M	133	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	P	149	ALA	CB-CA-C	-6.66	100.11	110.10
1	F	291	LEU	CB-CG-CD2	-6.66	99.68	111.00
1	F	326	ALA	N-CA-CB	-6.66	100.78	110.10
1	B	14	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	H	345	THR	C-N-CA	6.65	136.27	122.30
1	L	298	SER	N-CA-CB	-6.65	100.53	110.50
1	A	160	SER	N-CA-CB	-6.65	100.53	110.50
1	L	210	ALA	CB-CA-C	6.65	120.07	110.10
1	N	143	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	N	68	SER	O-C-N	-6.64	112.07	122.70
1	H	185	ILE	O-C-N	-6.64	112.07	122.70
1	Q	213	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	N	108	LEU	CB-CG-CD2	-6.64	99.71	111.00
1	D	124	ILE	O-C-N	-6.64	112.08	122.70
1	D	249	ALA	CB-CA-C	6.64	120.05	110.10
1	L	300	SER	N-CA-CB	6.64	120.45	110.50
1	B	336	GLN	O-C-N	6.63	133.31	122.70
1	B	164	GLN	CB-CG-CD	6.63	128.84	111.60
1	E	24	ALA	CA-C-N	6.63	131.78	117.20
1	A	169	ALA	O-C-N	6.63	133.30	122.70
1	L	234	THR	CA-CB-CG2	6.63	121.68	112.40
1	L	155	ASP	CB-CG-OD1	6.62	124.26	118.30
1	K	118	THR	N-CA-CB	-6.62	97.72	110.30
1	Q	118	THR	CA-CB-CG2	-6.62	103.13	112.40
1	D	244	THR	N-CA-CB	-6.62	97.73	110.30
1	L	151	LEU	CD1-CG-CD2	-6.62	90.65	110.50
1	K	66	ASP	N-CA-CB	-6.62	98.69	110.60
1	N	65	VAL	CA-C-O	6.61	133.99	120.10
1	A	199	GLU	CB-CG-CD	6.61	132.05	114.20
1	F	24	ALA	CA-C-N	6.61	131.74	117.20
1	J	226	THR	N-CA-CB	-6.61	97.74	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	199	GLU	CA-CB-CG	6.61	127.94	113.40
1	N	303	ARG	CD-NE-CZ	-6.61	114.35	123.60
1	R	42	ARG	O-C-N	6.61	133.27	122.70
1	K	123	THR	CB-CA-C	-6.61	93.76	111.60
1	E	172	ARG	NH1-CZ-NH2	6.61	126.67	119.40
1	N	195	ASP	CA-CB-CG	-6.60	98.87	113.40
1	J	330	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	C	177	CYS	O-C-N	-6.59	112.15	122.70
1	M	277	GLU	CG-CD-OE1	6.59	131.49	118.30
1	O	133	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	P	258	ARG	N-CA-CB	6.59	122.47	110.60
1	R	3	ARG	CA-C-O	-6.59	106.26	120.10
1	Q	10	GLU	CA-C-O	-6.59	106.26	120.10
1	B	342	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	J	24	ALA	CA-C-O	-6.59	106.27	120.10
1	A	72	SER	O-C-N	6.58	133.23	122.70
1	R	244	THR	N-CA-CB	-6.58	97.80	110.30
1	E	303	ARG	CG-CD-NE	6.57	125.60	111.80
1	R	55	ARG	NH1-CZ-NH2	6.57	126.63	119.40
1	M	173	TYR	CB-CG-CD1	6.57	124.94	121.00
1	H	42	ARG	CD-NE-CZ	-6.56	114.41	123.60
1	J	22	ILE	CA-C-N	6.56	131.64	117.20
1	N	52	GLU	OE1-CD-OE2	-6.56	115.42	123.30
1	G	152	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	M	214	LYS	CD-CE-NZ	6.56	126.79	111.70
1	C	233	VAL	O-C-N	-6.56	112.20	122.70
1	E	350	ALA	N-CA-CB	-6.56	100.92	110.10
1	O	116	ALA	CB-CA-C	-6.56	100.27	110.10
1	D	98	LYS	CA-CB-CG	-6.55	98.98	113.40
1	P	206	GLU	OE1-CD-OE2	6.55	131.17	123.30
1	J	140	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	M	70	ASN	CA-C-O	-6.55	106.34	120.10
1	P	179	GLN	CA-CB-CG	6.55	127.81	113.40
1	D	56	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	L	148	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	E	72	SER	CB-CA-C	-6.54	97.67	110.10
1	A	45	ARG	CG-CD-NE	-6.54	98.06	111.80
1	E	352	SER	N-CA-CB	6.54	120.31	110.50
1	A	223	LEU	O-C-N	6.54	133.16	122.70
1	I	28	GLY	CA-C-O	6.54	132.37	120.60
1	O	255	ALA	N-CA-CB	-6.54	100.94	110.10
1	Q	155	ASP	CB-CG-OD1	-6.54	112.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	90	GLY	CA-C-O	-6.54	108.83	120.60
1	H	17	GLU	OE1-CD-OE2	6.54	131.14	123.30
1	D	38	THR	O-C-N	6.53	133.15	122.70
1	R	162	ALA	O-C-N	6.53	133.15	122.70
1	J	3	ARG	NH1-CZ-NH2	-6.53	112.22	119.40
1	J	330	ARG	NH1-CZ-NH2	6.53	126.58	119.40
1	K	24	ALA	C-N-CA	-6.53	105.38	121.70
1	L	80	HIS	CA-CB-CG	-6.53	102.50	113.60
1	R	99	GLU	OE1-CD-OE2	6.53	131.14	123.30
1	D	45	ARG	NH1-CZ-NH2	6.53	126.58	119.40
1	G	296	LYS	CB-CA-C	-6.53	97.34	110.40
1	I	328	MET	N-CA-CB	-6.53	98.85	110.60
1	N	207	LYS	CG-CD-CE	6.53	131.48	111.90
1	A	114	PRO	C-N-CA	6.53	138.01	121.70
1	J	258	ARG	CB-CA-C	-6.52	97.35	110.40
1	R	123	THR	N-CA-C	-6.52	93.39	111.00
1	L	118	THR	N-CA-CB	-6.52	97.91	110.30
1	N	79	PHE	CA-C-N	6.52	131.54	117.20
1	A	51	THR	N-CA-CB	-6.52	97.92	110.30
1	E	295	TRP	CB-CG-CD1	-6.52	118.53	127.00
1	D	3	ARG	CB-CA-C	6.51	123.43	110.40
1	A	238	ALA	C-N-CA	-6.51	105.42	121.70
1	O	338	ALA	N-CA-CB	6.51	119.22	110.10
1	P	325	GLU	CB-CG-CD	-6.51	96.62	114.20
1	C	3	ARG	CA-C-N	6.51	131.52	117.20
1	I	258	ARG	CG-CD-NE	-6.51	98.13	111.80
1	K	293	LYS	N-CA-CB	-6.51	98.89	110.60
1	D	56	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	N	82	THR	CA-CB-CG2	6.50	121.51	112.40
1	H	61	ILE	CA-CB-CG1	-6.50	98.65	111.00
1	B	268	CYS	O-C-N	6.50	133.10	122.70
1	D	285	ALA	CB-CA-C	-6.50	100.35	110.10
1	N	267	ILE	CB-CA-C	6.50	124.60	111.60
1	I	68	SER	C-N-CA	-6.50	105.46	121.70
1	M	134	CYS	O-C-N	-6.50	112.31	122.70
1	K	297	LEU	O-C-N	-6.50	112.31	122.70
1	L	6	ALA	CB-CA-C	-6.50	100.36	110.10
1	H	306	GLN	N-CA-CB	-6.49	98.91	110.60
1	N	171	ALA	N-CA-CB	6.49	119.19	110.10
1	P	90	GLY	O-C-N	6.49	133.09	122.70
1	D	301	TYR	CB-CG-CD2	6.49	124.89	121.00
1	H	329	LYS	CA-CB-CG	6.49	127.68	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	123	THR	CB-CA-C	-6.49	94.08	111.60
1	P	213	TYR	CB-CG-CD2	6.49	124.89	121.00
1	R	172	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	D	151	LEU	CA-C-N	6.49	131.47	117.20
1	J	199	GLU	CB-CG-CD	6.49	131.71	114.20
1	L	24	ALA	CA-C-N	6.49	131.47	117.20
1	O	326	ALA	N-CA-CB	-6.49	101.02	110.10
1	B	191	ILE	CG1-CB-CG2	-6.49	97.13	111.40
1	E	190	VAL	CA-CB-CG2	6.48	120.62	110.90
1	D	3	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
1	E	345	THR	N-CA-CB	6.48	122.61	110.30
1	D	75	GLY	CA-C-N	-6.48	102.95	117.20
1	J	167	ALA	N-CA-CB	-6.48	101.03	110.10
1	P	165	GLU	OE1-CD-OE2	6.47	131.07	123.30
1	C	265	PRO	C-N-CA	-6.47	108.71	122.30
1	D	151	LEU	CD1-CG-CD2	-6.47	91.08	110.50
1	H	197	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	I	195	ASP	CB-CA-C	-6.47	97.46	110.40
1	M	294	PRO	O-C-N	6.47	133.06	122.70
1	H	24	ALA	N-CA-CB	6.47	119.16	110.10
1	Q	325	GLU	OE1-CD-OE2	6.47	131.06	123.30
1	H	204	VAL	CA-CB-CG2	-6.46	101.20	110.90
1	M	248	VAL	CA-CB-CG2	-6.46	101.20	110.90
1	R	94	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	F	350	ALA	C-N-CA	6.46	137.85	121.70
1	P	330	ARG	CG-CD-NE	6.46	125.37	111.80
1	Q	10	GLU	O-C-N	6.46	133.03	122.70
1	J	87	ASP	CB-CG-OD2	6.45	124.11	118.30
1	N	237	HIS	CB-CA-C	-6.45	97.49	110.40
1	B	4	PHE	CB-CG-CD2	6.45	125.31	120.80
1	H	148	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	204	VAL	CA-CB-CG2	-6.45	101.23	110.90
1	G	89	GLN	CB-CA-C	-6.44	97.51	110.40
1	G	123	THR	CB-CA-C	-6.44	94.21	111.60
1	R	333	ALA	O-C-N	6.44	133.01	122.70
1	O	25	ASN	CA-CB-CG	6.44	127.57	113.40
1	O	208	VAL	CA-CB-CG1	-6.44	101.24	110.90
1	R	237	HIS	CB-CA-C	-6.44	97.52	110.40
1	P	123	THR	CB-CA-C	-6.44	94.21	111.60
1	I	341	GLN	CA-CB-CG	-6.44	99.24	113.40
1	K	195	ASP	N-CA-CB	-6.44	99.02	110.60
1	B	218	ASP	CB-CG-OD2	-6.43	112.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	195	ASP	N-CA-CB	-6.43	99.02	110.60
1	K	152	ARG	CB-CA-C	-6.43	97.54	110.40
1	N	11	GLN	O-C-N	6.43	132.99	122.70
1	A	199	GLU	CA-CB-CG	6.43	127.54	113.40
1	K	296	LYS	O-C-N	6.43	132.98	122.70
1	G	178	GLN	O-C-N	-6.43	112.42	122.70
1	M	137	TYR	CB-CG-CD1	6.43	124.86	121.00
1	O	160	SER	CB-CA-C	-6.43	97.89	110.10
1	G	152	ARG	CD-NE-CZ	-6.42	114.61	123.60
1	D	296	LYS	CB-CA-C	-6.42	97.56	110.40
1	I	271	SER	O-C-N	-6.42	112.28	123.20
1	I	332	MET	O-C-N	6.42	132.97	122.70
1	H	149	ALA	CB-CA-C	-6.42	100.47	110.10
1	B	71	GLN	CA-CB-CG	6.42	127.52	113.40
1	C	303	ARG	CD-NE-CZ	6.42	132.58	123.60
1	K	24	ALA	CA-C-N	6.42	131.32	117.20
1	O	66	ASP	CB-CG-OD1	6.42	124.08	118.30
1	P	94	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	J	199	GLU	CA-CB-CG	6.41	127.51	113.40
1	D	16	SER	CB-CA-C	6.41	122.28	110.10
1	G	76	VAL	CA-CB-CG2	-6.41	101.28	110.90
1	B	204	VAL	O-C-N	6.41	132.96	122.70
1	B	228	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	D	248	VAL	CA-CB-CG2	-6.41	101.29	110.90
1	B	3	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	B	333	ALA	O-C-N	6.41	132.95	122.70
1	D	151	LEU	CA-CB-CG	6.41	130.03	115.30
1	F	65	VAL	CG1-CB-CG2	-6.41	100.65	110.90
1	F	342	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	I	51	THR	CA-C-O	-6.40	106.65	120.10
1	L	104	VAL	CA-CB-CG2	-6.40	101.29	110.90
1	B	183	VAL	CA-CB-CG1	6.40	120.50	110.90
1	I	223	LEU	O-C-N	6.40	132.94	122.70
1	I	249	ALA	CB-CA-C	6.40	119.70	110.10
1	J	4	PHE	CG-CD2-CE2	6.40	127.84	120.80
1	N	330	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	G	152	ARG	NH1-CZ-NH2	6.39	126.43	119.40
1	R	101	GLY	O-C-N	-6.39	112.47	122.70
1	P	148	ARG	CA-C-O	-6.39	106.68	120.10
1	A	287	ASN	O-C-N	-6.39	112.48	122.70
1	G	213	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	Q	218	ASP	CB-CG-OD2	-6.39	112.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	73	ILE	O-C-N	-6.38	112.35	123.20
1	K	114	PRO	O-C-N	6.38	132.91	122.70
1	K	161	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	D	119	ASN	O-C-N	-6.38	112.49	122.70
1	K	212	VAL	CA-CB-CG2	-6.38	101.33	110.90
1	M	278	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	P	258	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
1	J	132	GLU	CG-CD-OE1	6.38	131.06	118.30
1	I	56	ARG	NH1-CZ-NH2	6.37	126.41	119.40
1	K	148	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	I	68	SER	CA-CB-OG	-6.37	94.00	111.20
1	M	151	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	B	56	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	Q	222	TYR	CB-CG-CD1	6.37	124.82	121.00
1	R	3	ARG	NH1-CZ-NH2	6.36	126.40	119.40
1	F	65	VAL	N-CA-CB	-6.36	97.51	111.50
1	L	87	ASP	CA-CB-CG	-6.35	99.42	113.40
1	F	284	ASN	CB-CG-OD1	6.35	134.30	121.60
1	I	132	GLU	CG-CD-OE1	6.35	131.00	118.30
1	N	89	GLN	CB-CA-C	-6.35	97.70	110.40
1	H	355	SER	N-CA-CB	6.35	120.02	110.50
1	G	10	GLU	CB-CG-CD	-6.34	97.07	114.20
1	I	191	ILE	N-CA-CB	-6.34	96.21	110.80
1	Q	249	ALA	O-C-N	-6.34	112.55	122.70
1	H	347	SER	N-CA-CB	6.34	120.01	110.50
1	N	305	LEU	C-N-CA	-6.34	105.85	121.70
1	O	342	TYR	CB-CG-CD1	6.34	124.81	121.00
1	F	156	GLN	CB-CG-CD	-6.34	95.12	111.60
1	E	160	SER	N-CA-CB	-6.34	100.99	110.50
1	O	187	GLU	CG-CD-OE2	6.34	130.97	118.30
1	B	34	GLU	CG-CD-OE1	6.33	130.96	118.30
1	J	109	ASP	OD1-CG-OD2	6.33	135.33	123.30
1	P	348	SER	CB-CA-C	6.33	122.12	110.10
1	R	217	ASN	OD1-CG-ND2	-6.33	107.35	121.90
1	P	262	ALA	O-C-N	-6.33	112.58	122.70
1	G	222	TYR	N-CA-CB	-6.32	99.22	110.60
1	G	299	PHE	O-C-N	-6.32	112.58	122.70
1	P	226	THR	N-CA-CB	-6.32	98.28	110.30
1	C	199	GLU	OE1-CD-OE2	-6.32	115.71	123.30
1	D	100	LYS	O-C-N	-6.32	112.45	123.20
1	D	158	PRO	N-CA-CB	-6.32	95.65	102.60
1	H	310	LEU	CA-CB-CG	6.32	129.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	303	ARG	CD-NE-CZ	-6.32	114.75	123.60
1	F	339	LYS	CA-CB-CG	6.32	127.30	113.40
1	O	97	LEU	O-C-N	-6.32	112.59	122.70
1	I	53	GLU	OE1-CD-OE2	6.31	130.88	123.30
1	C	59	ARG	NE-CZ-NH2	6.31	123.46	120.30
1	H	51	THR	N-CA-CB	-6.31	98.31	110.30
1	B	226	THR	CA-CB-OG1	-6.31	95.75	109.00
1	I	34	GLU	CA-CB-CG	6.31	127.28	113.40
1	Q	187	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	D	89	GLN	CB-CG-CD	-6.31	95.20	111.60
1	E	295	TRP	CA-C-O	-6.31	106.86	120.10
1	E	2	HIS	CA-C-N	6.30	131.07	117.20
1	N	186	VAL	N-CA-CB	-6.30	97.63	111.50
1	Q	8	THR	CA-CB-CG2	-6.30	103.57	112.40
1	C	244	THR	N-CA-CB	-6.30	98.33	110.30
1	D	152	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
1	P	179	GLN	OE1-CD-NE2	6.30	136.39	121.90
1	A	343	VAL	CB-CA-C	-6.30	99.43	111.40
1	Q	150	VAL	O-C-N	6.30	132.78	122.70
1	E	45	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	136	GLN	CA-CB-CG	6.29	127.24	113.40
1	L	108	LEU	CB-CG-CD2	-6.29	100.30	111.00
1	G	47	LYS	C-N-CA	6.29	137.43	121.70
1	I	265	PRO	C-N-CA	-6.29	109.09	122.30
1	M	69	ILE	CA-CB-CG1	6.29	122.95	111.00
1	R	33	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	B	118	THR	CA-CB-CG2	6.29	121.20	112.40
1	H	213	TYR	CG-CD1-CE1	6.29	126.33	121.30
1	D	348	SER	CA-C-O	6.29	133.30	120.10
1	K	191	ILE	N-CA-CB	-6.29	96.34	110.80
1	D	237	HIS	CA-CB-CG	-6.29	102.91	113.60
1	B	218	ASP	CA-C-N	-6.28	103.38	117.20
1	C	182	LEU	O-C-N	-6.28	112.65	122.70
1	D	308	SER	CB-CA-C	6.28	122.04	110.10
1	E	308	SER	CB-CA-C	6.28	122.04	110.10
1	L	212	VAL	CA-CB-CG1	-6.28	101.47	110.90
1	M	24	ALA	N-CA-CB	6.28	118.90	110.10
1	D	164	GLN	CB-CG-CD	6.28	127.93	111.60
1	C	195	ASP	CB-CA-C	-6.28	97.84	110.40
1	J	76	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	L	148	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
1	R	149	ALA	CB-CA-C	-6.28	100.68	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	166	ASN	CB-CG-ND2	6.28	131.77	116.70
1	I	341	GLN	C-N-CA	-6.28	106.01	121.70
1	K	325	GLU	CB-CG-CD	-6.28	97.26	114.20
1	H	89	GLN	N-CA-CB	-6.27	99.31	110.60
1	J	118	THR	N-CA-CB	-6.27	98.38	110.30
1	M	118	THR	CA-CB-CG2	6.27	121.18	112.40
1	J	344	HIS	CA-CB-CG	-6.27	102.94	113.60
1	H	81	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	K	348	SER	C-N-CA	-6.27	109.13	122.30
1	O	261	PRO	CA-C-O	6.27	135.25	120.20
1	G	258	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	P	35	SER	O-C-N	6.27	132.73	122.70
1	B	218	ASP	OD1-CG-OD2	6.27	135.21	123.30
1	J	113	ALA	N-CA-CB	6.26	118.87	110.10
1	R	276	GLU	N-CA-CB	6.26	121.87	110.60
1	F	248	VAL	CA-CB-CG2	-6.26	101.51	110.90
1	O	307	ALA	N-CA-CB	-6.26	101.33	110.10
1	L	210	ALA	N-CA-CB	-6.26	101.34	110.10
1	R	124	ILE	CB-CG1-CD1	6.26	131.43	113.90
1	H	226	THR	N-CA-CB	-6.26	98.41	110.30
1	J	53	GLU	CG-CD-OE1	6.26	130.81	118.30
1	F	218	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	F	68	SER	CA-CB-OG	6.25	128.08	111.20
1	N	3	ARG	CG-CD-NE	6.25	124.93	111.80
1	O	80	HIS	CB-CA-C	-6.25	97.90	110.40
1	I	25	ASN	C-N-CA	-6.25	109.19	122.30
1	C	206	GLU	CG-CD-OE1	6.24	130.79	118.30
1	N	94	ARG	CA-CB-CG	6.24	127.14	113.40
1	G	56	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	J	51	THR	CA-CB-CG2	6.24	121.14	112.40
1	A	216	LEU	CA-CB-CG	6.24	129.65	115.30
1	J	4	PHE	N-CA-CB	-6.24	99.37	110.60
1	Q	25	ASN	CA-CB-CG	6.24	127.13	113.40
1	D	226	THR	CA-C-O	-6.24	107.00	120.10
1	I	68	SER	N-CA-C	-6.24	94.16	111.00
1	J	209	LEU	CB-CG-CD2	-6.24	100.40	111.00
1	F	33	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	L	289	CYS	CB-CA-C	-6.24	97.93	110.40
1	L	3	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	E	258	ARG	CG-CD-NE	-6.23	98.71	111.80
1	R	265	PRO	C-N-CA	-6.23	109.21	122.30
1	K	60	GLU	O-C-N	6.23	132.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	70	ASN	N-CA-C	-6.23	94.18	111.00
1	R	191	ILE	CB-CG1-CD1	-6.23	96.45	113.90
1	E	301	TYR	CD1-CE1-CZ	-6.23	114.19	119.80
1	C	248	VAL	CA-CB-CG2	-6.23	101.56	110.90
1	I	26	GLY	C-N-CA	-6.23	106.13	121.70
1	I	150	VAL	C-N-CA	6.23	137.27	121.70
1	N	344	HIS	CA-CB-CG	-6.23	103.01	113.60
1	E	226	THR	CA-CB-OG1	-6.23	95.93	109.00
1	B	283	LEU	CB-CG-CD1	6.22	121.58	111.00
1	E	119	ASN	O-C-N	-6.22	112.74	122.70
1	P	42	ARG	NH1-CZ-NH2	-6.22	112.55	119.40
1	Q	74	GLY	C-N-CA	-6.22	109.23	122.30
1	E	19	ALA	CB-CA-C	-6.22	100.77	110.10
1	L	244	THR	N-CA-CB	-6.22	98.48	110.30
1	E	137	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	Q	89	GLN	O-C-N	-6.22	112.62	123.20
1	R	4	PHE	CB-CA-C	-6.22	97.96	110.40
1	F	123	THR	CB-CA-C	-6.22	94.81	111.60
1	O	147	TRP	CZ3-CH2-CZ2	-6.22	114.14	121.60
1	F	42	ARG	NH1-CZ-NH2	-6.22	112.56	119.40
1	J	33	ASP	CB-CG-OD2	6.22	123.89	118.30
1	N	165	GLU	CG-CD-OE2	-6.21	105.88	118.30
1	Q	190	VAL	C-N-CA	6.21	137.23	121.70
1	B	240	THR	CA-C-O	-6.21	107.07	120.10
1	K	277	GLU	CG-CD-OE1	6.20	130.70	118.30
1	K	309	ALA	CA-C-O	6.20	133.12	120.10
1	P	79	PHE	CB-CG-CD1	-6.20	116.46	120.80
1	Q	130	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	O	180	ASN	O-C-N	-6.20	112.67	123.20
1	P	344	HIS	N-CA-CB	6.20	121.75	110.60
1	D	135	ALA	O-C-N	6.19	132.61	122.70
1	E	187	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	K	342	TYR	CB-CG-CD2	6.19	124.72	121.00
1	R	67	SER	N-CA-CB	-6.19	101.21	110.50
1	R	224	GLU	CG-CD-OE2	6.19	130.67	118.30
1	I	22	ILE	CA-C-O	-6.18	107.11	120.10
1	A	24	ALA	N-CA-CB	6.18	118.76	110.10
1	B	81	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	D	99	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	M	10	GLU	CA-CB-CG	6.18	127.00	113.40
1	R	214	LYS	CB-CA-C	-6.18	98.03	110.40
1	M	90	GLY	CA-C-O	-6.18	109.47	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	THR	N-CA-CB	-6.18	98.56	110.30
1	B	132	GLU	CG-CD-OE1	6.18	130.66	118.30
1	F	71	GLN	O-C-N	6.18	132.59	122.70
1	J	300	SER	O-C-N	6.18	132.59	122.70
1	A	343	VAL	CA-C-N	-6.18	103.61	117.20
1	G	246	GLU	O-C-N	-6.18	112.81	122.70
1	K	101	GLY	CA-C-O	-6.18	109.48	120.60
1	R	94	ARG	NH1-CZ-NH2	6.17	126.19	119.40
1	H	4	PHE	N-CA-C	-6.17	94.33	111.00
1	J	219	HIS	CG-ND1-CE1	6.17	116.84	108.20
1	E	109	ASP	N-CA-CB	6.17	121.71	110.60
1	O	87	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	282	ASN	CB-CG-OD1	-6.17	109.26	121.60
1	D	149	ALA	N-CA-CB	6.17	118.73	110.10
1	M	69	ILE	CA-C-O	6.17	133.05	120.10
1	N	237	HIS	CA-CB-CG	-6.17	103.11	113.60
1	I	11	GLN	O-C-N	6.17	132.57	122.70
1	P	352	SER	CA-C-N	-6.17	103.63	117.20
1	I	34	GLU	OE1-CD-OE2	6.17	130.70	123.30
1	O	10	GLU	CB-CA-C	-6.17	98.07	110.40
1	Q	87	ASP	CB-CA-C	-6.16	98.07	110.40
1	A	168	ASN	O-C-N	6.16	132.56	122.70
1	G	344	HIS	CA-C-O	6.16	133.04	120.10
1	N	328	MET	N-CA-CB	-6.16	99.51	110.60
1	J	24	ALA	O-C-N	-6.16	112.85	122.70
1	N	98	LYS	CD-CE-NZ	6.16	125.86	111.70
1	H	60	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	I	25	ASN	N-CA-CB	6.16	121.68	110.60
1	D	148	ARG	CG-CD-NE	6.15	124.72	111.80
1	J	152	ARG	CA-CB-CG	6.15	126.94	113.40
1	P	357	PHE	CA-CB-CG	6.15	128.66	113.90
1	G	302	GLY	O-C-N	-6.15	112.86	122.70
1	L	56	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	C	151	LEU	CA-CB-CG	-6.15	101.16	115.30
1	J	345	THR	N-CA-C	6.15	127.60	111.00
1	L	56	ARG	CD-NE-CZ	-6.15	115.00	123.60
1	R	45	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	E	160	SER	O-C-N	-6.15	112.87	122.70
1	G	121	GLU	OE1-CD-OE2	6.14	130.67	123.30
1	Q	113	ALA	CB-CA-C	6.14	119.31	110.10
1	C	136	GLN	CG-CD-OE1	6.14	133.88	121.60
1	F	32	ALA	N-CA-CB	-6.14	101.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	150	VAL	O-C-N	-6.14	112.88	122.70
1	J	89	GLN	CB-CG-CD	-6.14	95.64	111.60
1	C	3	ARG	CG-CD-NE	6.14	124.69	111.80
1	D	90	GLY	O-C-N	6.14	132.52	122.70
1	N	191	ILE	CA-CB-CG1	-6.13	99.35	111.00
1	N	274	MET	CA-CB-CG	-6.13	102.88	113.30
1	F	148	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	N	164	GLN	CB-CG-CD	6.13	127.54	111.60
1	Q	213	TYR	CB-CG-CD1	6.13	124.68	121.00
1	E	156	GLN	O-C-N	-6.13	112.90	122.70
1	I	147	TRP	O-C-N	6.13	132.51	122.70
1	O	221	VAL	CA-CB-CG2	-6.13	101.71	110.90
1	K	226	THR	N-CA-CB	-6.12	98.66	110.30
1	L	256	LEU	C-N-CA	-6.12	106.39	121.70
1	B	183	VAL	N-CA-C	-6.12	94.48	111.00
1	J	346	GLY	N-CA-C	-6.12	97.81	113.10
1	D	227	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	F	69	ILE	CA-CB-CG1	6.12	122.62	111.00
1	G	9	GLN	CG-CD-NE2	6.11	131.37	116.70
1	M	264	VAL	CA-CB-CG1	-6.11	101.73	110.90
1	B	226	THR	CA-CB-CG2	6.11	120.96	112.40
1	C	52	GLU	OE1-CD-OE2	-6.11	115.97	123.30
1	O	261	PRO	CA-C-N	-6.11	103.76	117.20
1	I	32	ALA	N-CA-CB	-6.11	101.55	110.10
1	D	2	HIS	CA-CB-CG	-6.11	103.22	113.60
1	H	332	MET	O-C-N	-6.11	112.93	122.70
1	P	234	THR	O-C-N	6.11	132.47	122.70
1	I	70	ASN	OD1-CG-ND2	-6.11	107.86	121.90
1	K	87	ASP	CB-CG-OD2	6.11	123.80	118.30
1	Q	72	SER	N-CA-CB	-6.10	101.34	110.50
1	B	319	ASN	CA-CB-CG	-6.10	99.98	113.40
1	D	59	ARG	CA-CB-CG	-6.10	99.98	113.40
1	H	132	GLU	N-CA-CB	6.10	121.58	110.60
1	P	358	THR	CA-CB-CG2	6.10	120.94	112.40
1	A	66	ASP	C-N-CA	6.10	136.95	121.70
1	A	118	THR	C-N-CA	-6.10	106.46	121.70
1	D	264	VAL	CA-C-O	-6.09	107.30	120.10
1	B	148	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	G	214	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	Q	190	VAL	CA-CB-CG1	-6.09	101.76	110.90
1	D	279	ALA	N-CA-CB	6.09	118.62	110.10
1	E	216	LEU	CA-CB-CG	6.09	129.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	100	LYS	CB-CA-C	-6.09	98.22	110.40
1	J	173	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	O	109	ASP	O-C-N	-6.09	112.96	122.70
1	I	55	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	I	133	ARG	CG-CD-NE	6.08	124.57	111.80
1	O	300	SER	N-CA-CB	6.08	119.62	110.50
1	I	123	THR	N-CA-CB	6.08	121.85	110.30
1	I	168	ASN	O-C-N	6.08	132.43	122.70
1	L	24	ALA	CA-C-O	-6.08	107.33	120.10
1	O	42	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	O	164	GLN	CB-CG-CD	6.08	127.41	111.60
1	E	12	LYS	CD-CE-NZ	-6.08	97.73	111.70
1	H	107	LYS	CG-CD-CE	6.08	130.12	111.90
1	A	259	THR	O-C-N	-6.07	112.98	122.70
1	H	42	ARG	O-C-N	6.07	132.42	122.70
1	B	344	HIS	O-C-N	6.07	132.42	122.70
1	H	190	VAL	C-N-CA	6.07	136.88	121.70
1	A	348	SER	CA-C-O	-6.07	107.36	120.10
1	B	93	PHE	CZ-CE2-CD2	6.07	127.38	120.10
1	J	224	GLU	CA-CB-CG	6.07	126.75	113.40
1	P	156	GLN	CA-CB-CG	-6.07	100.05	113.40
1	O	289	CYS	CB-CA-C	-6.07	98.27	110.40
1	C	295	TRP	CD1-NE1-CE2	-6.06	103.54	109.00
1	L	237	HIS	CA-CB-CG	-6.06	103.29	113.60
1	A	128	ASP	O-C-N	-6.06	112.90	123.20
1	D	211	ALA	N-CA-CB	-6.06	101.61	110.10
1	O	204	VAL	CA-CB-CG1	-6.06	101.81	110.90
1	F	240	THR	O-C-N	6.06	132.39	122.70
1	R	216	LEU	CA-CB-CG	6.06	129.23	115.30
1	L	330	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	A	152	ARG	CB-CA-C	-6.05	98.30	110.40
1	C	2	HIS	CA-CB-CG	-6.05	103.31	113.60
1	B	243	TYR	C-N-CA	6.05	136.82	121.70
1	F	110	GLN	OE1-CD-NE2	6.05	135.81	121.90
1	H	99	GLU	CG-CD-OE2	-6.05	106.21	118.30
1	B	6	ALA	N-CA-CB	6.04	118.56	110.10
1	J	26	GLY	CA-C-O	-6.04	109.72	120.60
1	L	89	GLN	CB-CG-CD	-6.04	95.88	111.60
1	C	226	THR	CA-CB-CG2	6.04	120.86	112.40
1	F	138	LYS	CA-CB-CG	6.04	126.69	113.40
1	N	45	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	K	66	ASP	CA-CB-CG	6.04	126.68	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	51	THR	N-CA-CB	-6.04	98.83	110.30
1	M	352	SER	CB-CA-C	6.04	121.57	110.10
1	O	267	ILE	CA-CB-CG2	6.04	122.97	110.90
1	K	353	THR	N-CA-CB	-6.03	98.84	110.30
1	M	42	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
1	I	79	PHE	CB-CG-CD2	6.03	125.02	120.80
1	R	109	ASP	CB-CG-OD1	6.03	123.73	118.30
1	H	3	ARG	CB-CA-C	-6.03	98.34	110.40
1	F	353	THR	N-CA-C	-6.03	94.73	111.00
1	D	131	SER	N-CA-CB	6.02	119.54	110.50
1	G	181	GLY	CA-C-O	-6.02	109.76	120.60
1	P	296	LYS	O-C-N	6.02	132.34	122.70
1	C	170	LEU	O-C-N	6.02	132.33	122.70
1	P	59	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	G	41	ASN	O-C-N	6.02	132.33	122.70
1	J	1	ALA	CA-C-N	6.02	130.44	117.20
1	C	164	GLN	CB-CG-CD	6.01	127.24	111.60
1	E	343	VAL	N-CA-CB	6.01	124.73	111.50
1	A	27	LYS	N-CA-CB	-6.01	99.78	110.60
1	D	270	LEU	CB-CG-CD2	6.01	121.22	111.00
1	D	60	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	D	250	MET	CA-CB-CG	6.01	123.51	113.30
1	F	59	ARG	CA-CB-CG	-6.01	100.18	113.40
1	K	137	TYR	CB-CG-CD2	6.01	124.60	121.00
1	P	185	ILE	CA-C-N	6.01	130.41	117.20
1	B	281	LEU	N-CA-CB	-6.00	98.39	110.40
1	E	135	ALA	O-C-N	-6.00	113.09	122.70
1	O	200	HIS	CA-CB-CG	6.00	123.81	113.60
1	P	56	ARG	CD-NE-CZ	6.00	132.00	123.60
1	B	219	HIS	CA-C-N	-6.00	104.00	117.20
1	H	65	VAL	CG1-CB-CG2	-6.00	101.30	110.90
1	G	109	ASP	OD1-CG-OD2	6.00	134.69	123.30
1	D	295	TRP	N-CA-CB	-5.99	99.81	110.60
1	D	355	SER	N-CA-CB	5.99	119.49	110.50
1	I	164	GLN	CA-CB-CG	5.99	126.59	113.40
1	Q	225	GLY	CA-C-N	-5.99	104.02	117.20
1	E	183	VAL	CA-CB-CG2	5.99	119.89	110.90
1	A	274	MET	CA-CB-CG	5.99	123.48	113.30
1	C	172	ARG	NH1-CZ-NH2	5.99	125.99	119.40
1	K	164	GLN	CA-CB-CG	5.99	126.58	113.40
1	A	23	VAL	CG1-CB-CG2	-5.99	101.32	110.90
1	M	89	GLN	OE1-CD-NE2	5.99	135.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	195	ASP	N-CA-CB	-5.98	99.83	110.60
1	I	71	GLN	OE1-CD-NE2	5.98	135.66	121.90
1	K	249	ALA	CB-CA-C	5.98	119.07	110.10
1	P	82	THR	CA-C-N	5.98	130.36	117.20
1	E	15	LEU	O-C-N	-5.97	113.14	122.70
1	E	237	HIS	CB-CA-C	-5.97	98.45	110.40
1	I	291	LEU	CA-C-O	-5.97	107.55	120.10
1	K	166	ASN	CA-CB-CG	-5.97	100.25	113.40
1	K	218	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	N	259	THR	O-C-N	-5.97	113.14	122.70
1	M	301	TYR	CG-CD1-CE1	5.97	126.08	121.30
1	B	326	ALA	N-CA-CB	-5.97	101.75	110.10
1	P	309	ALA	N-CA-CB	5.97	118.46	110.10
1	D	132	GLU	CB-CG-CD	5.96	130.30	114.20
1	O	81	GLU	CA-CB-CG	5.96	126.52	113.40
1	F	151	LEU	CA-CB-CG	5.96	129.01	115.30
1	M	14	GLU	C-N-CA	-5.96	106.79	121.70
1	K	183	VAL	CA-CB-CG2	-5.96	101.96	110.90
1	L	66	ASP	CB-CG-OD1	5.96	123.66	118.30
1	O	51	THR	N-CA-CB	-5.96	98.98	110.30
1	P	72	SER	CB-CA-C	-5.96	98.78	110.10
1	E	140	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	F	90	GLY	C-N-CA	-5.96	106.81	121.70
1	R	198	LEU	CB-CG-CD2	5.96	121.13	111.00
1	B	85	GLN	CA-C-O	5.96	132.61	120.10
1	A	152	ARG	CB-CG-CD	5.95	127.08	111.60
1	M	189	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	R	65	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	D	70	ASN	N-CA-CB	-5.95	99.89	110.60
1	A	27	LYS	CD-CE-NZ	5.95	125.38	111.70
1	B	128	ASP	CB-CG-OD2	5.95	123.65	118.30
1	N	218	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	Q	24	ALA	CB-CA-C	-5.95	101.18	110.10
1	Q	341	GLN	CA-CB-CG	-5.95	100.31	113.40
1	C	216	LEU	CA-CB-CG	5.95	128.98	115.30
1	O	226	THR	N-CA-CB	-5.95	99.00	110.30
1	B	187	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	G	118	THR	C-N-CA	-5.94	106.84	121.70
1	D	29	ILE	CB-CG1-CD1	-5.94	97.27	113.90
1	E	213	TYR	CA-CB-CG	-5.94	102.11	113.40
1	H	173	TYR	CG-CD2-CE2	5.94	126.05	121.30
1	Q	3	ARG	CB-CA-C	5.93	122.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	321	GLU	OE1-CD-OE2	5.93	130.42	123.30
1	E	10	GLU	CB-CA-C	5.93	122.27	110.40
1	C	342	TYR	CB-CG-CD2	5.93	124.56	121.00
1	O	136	GLN	CB-CA-C	5.93	122.26	110.40
1	F	225	GLY	CA-C-N	-5.93	104.16	117.20
1	N	123	THR	CB-CA-C	-5.93	95.60	111.60
1	Q	258	ARG	CA-CB-CG	5.93	126.44	113.40
1	D	3	ARG	CG-CD-NE	5.92	124.24	111.80
1	G	89	GLN	CB-CG-CD	-5.92	96.20	111.60
1	I	104	VAL	CG1-CB-CG2	-5.92	101.42	110.90
1	A	165	GLU	O-C-N	-5.92	113.23	122.70
1	M	283	LEU	O-C-N	-5.92	113.23	122.70
1	G	250	MET	CB-CG-SD	5.92	130.16	112.40
1	L	94	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	F	344	HIS	CA-C-O	5.92	132.52	120.10
1	E	233	VAL	C-N-CA	5.91	136.48	121.70
1	O	203	TYR	CB-CG-CD2	5.91	124.55	121.00
1	Q	218	ASP	O-C-N	-5.91	113.24	122.70
1	L	125	GLN	CG-CD-OE1	5.91	133.42	121.60
1	J	137	TYR	CB-CG-CD1	5.91	124.55	121.00
1	M	51	THR	N-CA-CB	-5.91	99.07	110.30
1	D	121	GLU	CG-CD-OE2	-5.91	106.49	118.30
1	G	118	THR	CA-CB-CG2	-5.90	104.13	112.40
1	G	330	ARG	C-N-CA	-5.90	106.94	121.70
1	I	122	THR	OG1-CB-CG2	-5.90	96.42	110.00
1	O	49	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	J	217	ASN	CB-CG-ND2	-5.90	102.54	116.70
1	A	147	TRP	CE3-CZ3-CH2	-5.90	114.71	121.20
1	B	342	TYR	N-CA-CB	5.90	121.22	110.60
1	F	329	LYS	CD-CE-NZ	5.90	125.26	111.70
1	I	250	MET	O-C-N	5.90	132.13	122.70
1	O	132	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	R	87	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	10	GLU	CB-CA-C	-5.89	98.61	110.40
1	F	120	LYS	CA-CB-CG	-5.89	100.44	113.40
1	F	95	ASN	CA-CB-CG	-5.89	100.44	113.40
1	M	165	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	O	219	HIS	CA-C-O	5.89	132.47	120.10
1	C	94	ARG	CG-CD-NE	5.89	124.17	111.80
1	G	291	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	97	LEU	O-C-N	-5.88	113.28	122.70
1	B	276	GLU	OE1-CD-OE2	-5.88	116.24	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	GLN	C-N-CA	5.88	136.41	121.70
1	P	222	TYR	CB-CG-CD1	5.88	124.53	121.00
1	R	118	THR	N-CA-CB	-5.88	99.13	110.30
1	Q	330	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	F	59	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	G	55	ARG	CG-CD-NE	5.87	124.13	111.80
1	H	147	TRP	CA-CB-CG	5.87	124.86	113.70
1	F	152	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	P	343	VAL	CG1-CB-CG2	5.87	120.30	110.90
1	D	65	VAL	N-CA-CB	-5.87	98.59	111.50
1	G	23	VAL	CG1-CB-CG2	-5.87	101.51	110.90
1	K	232	MET	O-C-N	5.87	132.08	122.70
1	O	233	VAL	CA-CB-CG1	-5.87	102.10	110.90
1	Q	250	MET	CA-CB-CG	-5.87	103.33	113.30
1	B	89	GLN	CA-CB-CG	-5.86	100.50	113.40
1	O	159	SER	CA-C-O	5.86	132.41	120.10
1	B	93	PHE	CD1-CE1-CZ	5.86	127.13	120.10
1	K	4	PHE	N-CA-CB	-5.86	100.05	110.60
1	D	237	HIS	CB-CG-ND1	5.86	137.84	123.20
1	L	78	LEU	O-C-N	5.86	132.07	122.70
1	L	91	LYS	O-C-N	5.86	132.07	122.70
1	L	198	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	M	195	ASP	N-CA-CB	-5.86	100.06	110.60
1	M	219	HIS	CA-CB-CG	5.86	123.56	113.60
1	B	214	LYS	CA-C-O	5.85	132.39	120.10
1	B	225	GLY	CA-C-N	-5.85	104.33	117.20
1	D	346	GLY	CA-C-O	5.85	131.14	120.60
1	J	27	LYS	CA-CB-CG	-5.85	100.53	113.40
1	C	150	VAL	O-C-N	-5.85	113.34	122.70
1	R	183	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	J	344	HIS	CB-CA-C	5.85	122.09	110.40
1	Q	3	ARG	N-CA-C	-5.85	95.21	111.00
1	E	273	GLY	O-C-N	-5.85	113.35	122.70
1	Q	143	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	C	107	LYS	CA-C-N	5.84	130.06	117.20
1	I	77	ILE	O-C-N	5.84	132.05	122.70
1	E	342	TYR	N-CA-CB	5.84	121.11	110.60
1	G	2	HIS	N-CA-CB	5.84	121.11	110.60
1	I	187	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	N	272	GLY	C-N-CA	-5.84	110.04	122.30
1	R	218	ASP	O-C-N	-5.84	113.36	122.70
1	O	131	SER	N-CA-CB	5.84	119.26	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLU	CA-C-O	5.84	132.36	120.10
1	P	90	GLY	C-N-CA	-5.83	107.11	121.70
1	N	137	TYR	CB-CG-CD1	5.83	124.50	121.00
1	A	277	GLU	CG-CD-OE1	5.83	129.96	118.30
1	J	303	ARG	CD-NE-CZ	-5.83	115.44	123.60
1	O	70	ASN	CB-CA-C	-5.83	98.74	110.40
1	C	298	SER	N-CA-CB	-5.83	101.75	110.50
1	L	51	THR	N-CA-CB	-5.83	99.22	110.30
1	R	293	LYS	CD-CE-NZ	5.83	125.11	111.70
1	F	144	PHE	N-CA-CB	5.83	121.09	110.60
1	J	89	GLN	CG-CD-OE1	-5.82	109.95	121.60
1	K	357	PHE	CB-CA-C	-5.82	98.75	110.40
1	G	143	ASP	CB-CG-OD2	5.82	123.54	118.30
1	O	257	HIS	CA-C-O	-5.82	107.87	120.10
1	A	56	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	P	356	LEU	CB-CG-CD1	5.82	120.89	111.00
1	I	215	ALA	O-C-N	5.82	132.01	122.70
1	K	257	HIS	CA-CB-CG	5.82	123.49	113.60
1	C	292	PRO	O-C-N	-5.82	113.40	122.70
1	P	189	GLU	CG-CD-OE1	5.82	129.93	118.30
1	A	277	GLU	CG-CD-OE2	-5.81	106.67	118.30
1	L	329	LYS	CG-CD-CE	5.81	129.34	111.90
1	G	3	ARG	O-C-N	-5.81	113.41	122.70
1	F	172	ARG	NH1-CZ-NH2	5.81	125.79	119.40
1	P	237	HIS	O-C-N	-5.81	113.41	122.70
1	G	98	LYS	CB-CA-C	-5.80	98.79	110.40
1	M	161	LEU	CB-CG-CD1	5.80	120.87	111.00
1	R	140	ASP	OD1-CG-OD2	5.80	134.32	123.30
1	E	191	ILE	CB-CG1-CD1	-5.80	97.67	113.90
1	F	56	ARG	CG-CD-NE	5.80	123.97	111.80
1	I	11	GLN	C-N-CA	-5.80	107.21	121.70
1	A	109	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	L	114	PRO	N-CD-CG	-5.79	94.51	103.20
1	E	25	ASN	CA-CB-CG	5.79	126.14	113.40
1	R	141	GLY	O-C-N	5.79	131.97	122.70
1	C	33	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	D	282	ASN	CB-CG-OD1	-5.79	110.02	121.60
1	H	70	ASN	CA-CB-CG	-5.79	100.67	113.40
1	F	42	ARG	CG-CD-NE	5.79	123.95	111.80
1	F	190	VAL	O-C-N	-5.79	113.44	122.70
1	G	87	ASP	CA-CB-CG	-5.79	100.67	113.40
1	B	144	PHE	CB-CG-CD2	-5.78	116.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	GLU	CG-CD-OE1	5.78	129.87	118.30
1	E	327	PHE	O-C-N	-5.78	113.44	122.70
1	F	345	THR	N-CA-C	-5.78	95.39	111.00
1	R	33	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	F	189	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	J	308	SER	CB-CA-C	5.78	121.08	110.10
1	D	88	SER	CB-CA-C	5.78	121.08	110.10
1	D	229	LYS	CD-CE-NZ	-5.78	98.42	111.70
1	L	180	ASN	O-C-N	-5.78	113.38	123.20
1	Q	155	ASP	CB-CG-OD2	5.77	123.50	118.30
1	N	303	ARG	CB-CG-CD	5.77	126.61	111.60
1	D	265	PRO	C-N-CA	-5.77	110.18	122.30
1	H	152	ARG	CD-NE-CZ	-5.77	115.52	123.60
1	Q	309	ALA	N-CA-CB	5.77	118.18	110.10
1	E	50	ASN	O-C-N	5.77	131.93	122.70
1	E	195	ASP	CB-CA-C	-5.77	98.86	110.40
1	F	347	SER	CA-CB-OG	5.77	126.78	111.20
1	A	69	ILE	CA-CB-CG1	-5.77	100.04	111.00
1	B	346	GLY	C-N-CA	5.77	136.12	121.70
1	D	35	SER	N-CA-CB	-5.76	101.85	110.50
1	P	106	ILE	CB-CG1-CD1	-5.76	97.76	113.90
1	G	325	GLU	O-C-N	-5.76	113.48	122.70
1	D	92	LEU	O-C-N	-5.76	113.48	122.70
1	P	89	GLN	CB-CG-CD	-5.76	96.62	111.60
1	A	213	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	D	33	ASP	CA-C-O	-5.76	108.01	120.10
1	G	46	ILE	CB-CG1-CD1	5.76	130.02	113.90
1	D	155	ASP	CA-C-O	5.76	132.19	120.10
1	C	123	THR	N-CA-CB	5.75	121.23	110.30
1	H	172	ARG	O-C-N	-5.75	113.49	122.70
1	L	340	GLY	C-N-CA	-5.75	107.32	121.70
1	B	5	PRO	O-C-N	5.75	131.90	122.70
1	H	69	ILE	CA-CB-CG1	-5.75	100.08	111.00
1	I	336	GLN	CG-CD-OE1	5.75	133.09	121.60
1	H	27	LYS	O-C-N	-5.75	113.43	123.20
1	H	195	ASP	CB-CA-C	-5.75	98.91	110.40
1	F	69	ILE	CG1-CB-CG2	-5.74	98.77	111.40
1	G	84	TYR	CB-CG-CD2	5.74	124.45	121.00
1	M	27	LYS	CD-CE-NZ	5.74	124.91	111.70
1	C	51	THR	N-CA-CB	-5.74	99.39	110.30
1	Q	174	ALA	CB-CA-C	5.74	118.71	110.10
1	R	148	ARG	CA-C-O	5.74	132.16	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	124	ILE	CG1-CB-CG2	-5.74	98.77	111.40
1	K	258	ARG	CA-C-O	-5.74	108.04	120.10
1	D	71	GLN	CA-C-O	-5.74	108.05	120.10
1	Q	98	LYS	CB-CA-C	-5.74	98.92	110.40
1	Q	199	GLU	CA-CB-CG	5.74	126.03	113.40
1	B	218	ASP	N-CA-CB	-5.74	100.28	110.60
1	C	253	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	C	288	LEU	O-C-N	-5.73	113.53	122.70
1	N	165	GLU	N-CA-CB	-5.73	100.28	110.60
1	B	334	ASN	CA-C-O	-5.73	108.07	120.10
1	E	228	LEU	O-C-N	5.73	131.87	122.70
1	L	164	GLN	CB-CG-CD	5.73	126.50	111.60
1	E	116	ALA	N-CA-CB	5.73	118.12	110.10
1	A	259	THR	CA-C-N	5.73	129.80	117.20
1	A	31	ALA	O-C-N	5.72	131.86	122.70
1	C	188	PRO	N-CA-CB	5.72	110.17	103.30
1	L	121	GLU	OE1-CD-OE2	5.72	130.17	123.30
1	N	79	PHE	CA-C-O	-5.72	108.08	120.10
1	O	171	ALA	N-CA-CB	5.72	118.11	110.10
1	P	343	VAL	CA-CB-CG1	-5.72	102.32	110.90
1	G	222	TYR	CB-CG-CD1	5.72	124.43	121.00
1	J	294	PRO	O-C-N	5.72	131.85	122.70
1	M	226	THR	N-CA-CB	-5.72	99.43	110.30
1	O	126	GLY	C-N-CA	-5.72	107.40	121.70
1	A	300	SER	CA-C-O	-5.72	108.10	120.10
1	M	277	GLU	C-N-CA	-5.72	107.41	121.70
1	O	55	ARG	CD-NE-CZ	-5.72	115.60	123.60
1	B	280	THR	CA-CB-CG2	5.71	120.40	112.40
1	E	1	ALA	O-C-N	-5.71	113.56	122.70
1	E	213	TYR	CB-CG-CD1	5.71	124.43	121.00
1	L	260	VAL	CG1-CB-CG2	5.71	120.04	110.90
1	N	22	ILE	CA-C-O	-5.71	108.10	120.10
1	N	124	ILE	O-C-N	5.71	131.84	122.70
1	Q	123	THR	CB-CA-C	-5.71	96.17	111.60
1	C	295	TRP	CB-CA-C	-5.71	98.97	110.40
1	D	228	LEU	CA-C-O	-5.71	108.10	120.10
1	E	4	PHE	N-CA-C	-5.71	95.57	111.00
1	G	325	GLU	CA-C-O	5.71	132.09	120.10
1	O	111	GLY	CA-C-N	-5.71	104.78	116.20
1	Q	127	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	M	239	CYS	O-C-N	5.71	131.84	122.70
1	A	359	ALA	N-CA-CB	-5.71	102.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	218	ASP	N-CA-CB	-5.71	100.33	110.60
1	J	300	SER	N-CA-C	-5.71	95.59	111.00
1	L	258	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	O	270	LEU	C-N-CA	-5.71	107.44	121.70
1	B	219	HIS	CA-C-O	5.70	132.08	120.10
1	H	22	ILE	CA-C-O	-5.70	108.12	120.10
1	D	213	TYR	C-N-CA	-5.70	107.45	121.70
1	H	116	ALA	N-CA-CB	5.70	118.08	110.10
1	A	2	HIS	CA-C-O	5.70	132.07	120.10
1	B	333	ALA	CB-CA-C	5.70	118.65	110.10
1	E	204	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	K	89	GLN	OE1-CD-NE2	5.70	135.01	121.90
1	O	206	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	E	119	ASN	CA-C-O	5.70	132.07	120.10
1	O	237	HIS	CA-CB-CG	-5.70	103.91	113.60
1	F	172	ARG	CB-CA-C	-5.70	99.01	110.40
1	H	27	LYS	C-N-CA	5.70	134.26	122.30
1	H	190	VAL	O-C-N	-5.70	113.58	122.70
1	G	222	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	290	PRO	O-C-N	-5.69	113.59	122.70
1	E	153	ILE	CA-CB-CG1	-5.69	100.18	111.00
1	E	194	GLY	CA-C-O	5.69	130.85	120.60
1	H	8	THR	CA-CB-OG1	-5.69	97.05	109.00
1	K	217	ASN	CB-CG-OD1	5.69	132.98	121.60
1	L	301	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	P	343	VAL	CA-C-O	-5.69	108.15	120.10
1	R	3	ARG	N-CA-CB	5.69	120.84	110.60
1	B	17	GLU	CB-CA-C	5.69	121.78	110.40
1	H	173	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	A	49	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	A	287	ASN	CB-CG-OD1	5.69	132.98	121.60
1	B	307	ALA	CB-CA-C	-5.69	101.57	110.10
1	F	248	VAL	O-C-N	-5.69	113.60	122.70
1	I	175	SER	N-CA-CB	-5.69	101.97	110.50
1	J	336	GLN	O-C-N	5.69	131.80	122.70
1	Q	10	GLU	OE1-CD-OE2	5.69	130.12	123.30
1	R	155	ASP	CB-CG-OD1	5.69	123.42	118.30
1	H	82	THR	OG1-CB-CG2	5.69	123.08	110.00
1	J	133	ARG	NH1-CZ-NH2	5.69	125.65	119.40
1	N	128	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	N	87	ASP	N-CA-CB	-5.68	100.37	110.60
1	E	81	GLU	OE1-CD-OE2	-5.68	116.48	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	319	ASN	CA-CB-CG	-5.68	100.90	113.40
1	Q	3	ARG	CB-CG-CD	5.68	126.37	111.60
1	R	121	GLU	O-C-N	-5.68	113.61	122.70
1	C	104	VAL	CA-CB-CG2	-5.68	102.38	110.90
1	G	267	ILE	CA-CB-CG1	-5.68	100.21	111.00
1	I	164	GLN	CA-C-O	5.68	132.02	120.10
1	H	210	ALA	O-C-N	-5.68	113.62	122.70
1	C	56	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	E	66	ASP	CA-C-O	-5.67	108.19	120.10
1	E	87	ASP	OD1-CG-OD2	-5.67	112.52	123.30
1	F	347	SER	C-N-CA	5.67	135.89	121.70
1	D	186	VAL	CA-CB-CG2	-5.67	102.39	110.90
1	I	251	ALA	N-CA-CB	5.67	118.04	110.10
1	B	55	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	L	246	GLU	O-C-N	5.67	131.77	122.70
1	M	152	ARG	CA-CB-CG	5.67	125.88	113.40
1	N	224	GLU	CA-C-N	5.67	127.54	116.20
1	R	197	ASP	CB-CG-OD2	5.67	123.40	118.30
1	R	207	LYS	CA-CB-CG	5.67	125.88	113.40
1	H	321	GLU	OE1-CD-OE2	5.67	130.10	123.30
1	K	258	ARG	O-C-N	5.67	131.77	122.70
1	F	165	GLU	CG-CD-OE2	-5.67	106.97	118.30
1	L	24	ALA	N-CA-CB	5.67	118.03	110.10
1	G	218	ASP	OD1-CG-OD2	5.66	134.06	123.30
1	L	109	ASP	N-CA-CB	5.66	120.80	110.60
1	N	209	LEU	C-N-CA	-5.66	107.54	121.70
1	D	42	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
1	P	161	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	I	172	ARG	CA-CB-CG	-5.66	100.95	113.40
1	K	215	ALA	N-CA-CB	-5.66	102.18	110.10
1	N	132	GLU	CG-CD-OE1	5.66	129.62	118.30
1	P	208	VAL	CA-CB-CG2	-5.66	102.41	110.90
1	H	137	TYR	CA-CB-CG	5.66	124.15	113.40
1	C	1	ALA	CA-C-O	5.66	131.98	120.10
1	F	267	ILE	CB-CA-C	5.66	122.91	111.60
1	K	257	HIS	N-CA-CB	5.66	120.78	110.60
1	M	36	VAL	CA-CB-CG2	-5.65	102.42	110.90
1	Q	267	ILE	CG1-CB-CG2	-5.65	98.96	111.40
1	B	18	ILE	CA-C-N	-5.65	104.77	117.20
1	C	42	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
1	F	258	ARG	CA-CB-CG	5.65	125.84	113.40
1	I	93	PHE	N-CA-CB	-5.65	100.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	197	ASP	CB-CG-OD1	5.65	123.39	118.30
1	N	11	GLN	CG-CD-NE2	-5.65	103.14	116.70
1	A	218	ASP	C-N-CA	-5.65	107.58	121.70
1	Q	173	TYR	CB-CG-CD1	5.65	124.39	121.00
1	D	160	SER	O-C-N	5.64	131.73	122.70
1	E	226	THR	N-CA-CB	-5.64	99.57	110.30
1	E	342	TYR	O-C-N	5.64	131.73	122.70
1	I	134	CYS	O-C-N	-5.64	113.67	122.70
1	F	34	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	G	341	GLN	C-N-CA	-5.64	107.59	121.70
1	J	12	LYS	CA-CB-CG	-5.64	101.00	113.40
1	M	225	GLY	O-C-N	5.64	131.72	122.70
1	H	158	PRO	N-CA-CB	-5.64	96.40	102.60
1	F	133	ARG	CD-NE-CZ	-5.64	115.71	123.60
1	H	33	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	I	14	GLU	C-N-CA	-5.64	107.61	121.70
1	J	137	TYR	CZ-CE2-CD2	-5.64	114.73	119.80
1	L	81	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	O	147	TRP	CH2-CZ2-CE2	5.64	123.04	117.40
1	L	68	SER	N-CA-CB	-5.63	102.05	110.50
1	B	191	ILE	CB-CG1-CD1	-5.63	98.13	113.90
1	B	211	ALA	C-N-CA	-5.63	107.62	121.70
1	D	123	THR	N-CA-CB	5.63	121.00	110.30
1	D	210	ALA	CB-CA-C	5.63	118.55	110.10
1	L	81	GLU	N-CA-CB	5.63	120.73	110.60
1	R	33	ASP	OD1-CG-OD2	5.63	133.99	123.30
1	C	259	THR	CA-CB-CG2	-5.63	104.52	112.40
1	D	94	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	F	208	VAL	CA-CB-CG2	5.63	119.34	110.90
1	D	119	ASN	CB-CG-OD1	-5.62	110.35	121.60
1	B	25	ASN	CA-CB-CG	5.62	125.77	113.40
1	G	188	PRO	N-CA-C	-5.62	97.48	112.10
1	O	267	ILE	CB-CA-C	5.62	122.84	111.60
1	O	291	LEU	CB-CG-CD2	5.62	120.56	111.00
1	D	63	PHE	O-C-N	-5.62	113.71	122.70
1	D	199	GLU	CA-C-O	5.62	131.91	120.10
1	H	185	ILE	CA-C-N	5.62	129.57	117.20
1	R	76	VAL	CA-CB-CG1	-5.62	102.47	110.90
1	J	227	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	K	301	TYR	CA-CB-CG	5.62	124.08	113.40
1	M	124	ILE	N-CA-CB	-5.62	97.88	110.80
1	A	115	LEU	CA-C-O	5.62	131.90	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	227	LEU	N-CA-CB	5.62	121.64	110.40
1	I	42	ARG	CA-C-O	-5.62	108.30	120.10
1	N	110	GLN	C-N-CA	-5.62	110.50	122.30
1	E	75	GLY	N-CA-C	-5.62	99.06	113.10
1	F	78	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	F	144	PHE	CB-CG-CD1	-5.62	116.87	120.80
1	M	294	PRO	CA-C-O	-5.62	106.72	120.20
1	P	24	ALA	O-C-N	-5.62	113.71	122.70
1	D	21	SER	CA-C-O	-5.62	108.31	120.10
1	I	79	PHE	CB-CG-CD1	-5.62	116.87	120.80
1	I	111	GLY	CA-C-O	5.62	130.71	120.60
1	I	230	PRO	CB-CA-C	-5.62	97.96	112.00
1	D	191	ILE	CG1-CB-CG2	-5.61	99.05	111.40
1	J	66	ASP	CB-CG-OD1	5.61	123.35	118.30
1	K	98	LYS	CB-CG-CD	-5.61	97.00	111.60
1	P	228	LEU	O-C-N	5.61	131.68	122.70
1	C	30	LEU	O-C-N	5.61	131.68	122.70
1	B	116	ALA	O-C-N	5.61	132.74	123.20
1	A	152	ARG	CA-C-N	-5.61	104.86	117.20
1	M	195	ASP	CB-CA-C	-5.61	99.18	110.40
1	R	258	ARG	CB-CA-C	-5.61	99.18	110.40
1	A	344	HIS	N-CA-CB	-5.61	100.50	110.60
1	B	158	PRO	O-C-N	5.61	131.67	122.70
1	E	222	TYR	CA-CB-CG	5.61	124.05	113.40
1	O	226	THR	OG1-CB-CG2	5.61	122.90	110.00
1	L	152	ARG	CD-NE-CZ	-5.61	115.75	123.60
1	J	237	HIS	C-N-CA	-5.60	107.69	121.70
1	L	198	LEU	O-C-N	-5.60	113.73	122.70
1	N	11	GLN	C-N-CA	-5.60	107.69	121.70
1	Q	125	GLN	CA-CB-CG	5.60	125.73	113.40
1	K	287	ASN	CA-CB-CG	-5.60	101.08	113.40
1	F	174	ALA	CA-C-O	5.60	131.86	120.10
1	K	182	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	Q	148	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	240	THR	CA-CB-CG2	-5.60	104.56	112.40
1	C	303	ARG	CG-CD-NE	5.60	123.56	111.80
1	N	342	TYR	CG-CD2-CE2	5.60	125.78	121.30
1	A	156	GLN	CA-CB-CG	-5.60	101.09	113.40
1	E	348	SER	CA-C-O	5.60	131.85	120.10
1	Q	55	ARG	CD-NE-CZ	-5.60	115.77	123.60
1	F	156	GLN	CG-CD-OE1	-5.59	110.41	121.60
1	P	148	ARG	O-C-N	5.59	131.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	20	GLN	O-C-N	5.59	131.65	122.70
1	A	152	ARG	O-C-N	5.59	131.64	122.70
1	H	267	ILE	O-C-N	5.59	131.64	122.70
1	H	165	GLU	CB-CA-C	5.59	121.58	110.40
1	A	118	THR	CA-C-N	5.59	129.49	117.20
1	K	187	GLU	CA-CB-CG	5.58	125.69	113.40
1	L	56	ARG	NH1-CZ-NH2	5.58	125.54	119.40
1	B	175	SER	CB-CA-C	-5.58	99.49	110.10
1	F	116	ALA	CB-CA-C	5.58	118.47	110.10
1	O	207	LYS	CB-CA-C	5.58	121.57	110.40
1	A	241	LYS	CA-CB-CG	-5.58	101.12	113.40
1	A	287	ASN	CA-CB-CG	-5.58	101.12	113.40
1	C	71	GLN	OE1-CD-NE2	5.58	134.74	121.90
1	I	51	THR	CA-C-N	5.58	129.48	117.20
1	P	3	ARG	CD-NE-CZ	5.58	131.41	123.60
1	P	258	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	E	258	ARG	CB-CG-CD	5.58	126.11	111.60
1	P	30	LEU	O-C-N	5.58	131.63	122.70
1	E	51	THR	N-CA-CB	-5.58	99.70	110.30
1	E	175	SER	CB-CA-C	-5.58	99.51	110.10
1	G	186	VAL	O-C-N	-5.58	113.78	122.70
1	N	243	TYR	CB-CG-CD2	-5.58	117.66	121.00
1	O	311	ALA	N-CA-CB	-5.58	102.29	110.10
1	I	66	ASP	N-CA-CB	5.57	120.63	110.60
1	D	277	GLU	OE1-CD-OE2	-5.57	116.61	123.30
1	H	166	ASN	CB-CG-OD1	5.57	132.74	121.60
1	M	184	PRO	O-C-N	-5.57	113.79	122.70
1	L	26	GLY	C-N-CA	-5.57	107.78	121.70
1	R	60	GLU	OE1-CD-OE2	5.57	129.98	123.30
1	E	350	ALA	CA-C-O	5.57	131.79	120.10
1	M	260	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	B	213	TYR	C-N-CA	5.57	135.61	121.70
1	B	270	LEU	N-CA-C	-5.57	95.98	111.00
1	K	200	HIS	CB-CA-C	5.57	121.53	110.40
1	L	311	ALA	O-C-N	5.56	131.60	122.70
1	D	353	THR	CA-CB-CG2	-5.56	104.61	112.40
1	E	274	MET	CA-CB-CG	5.56	122.75	113.30
1	H	127	LEU	CB-CG-CD2	5.56	120.46	111.00
1	I	167	ALA	C-N-CA	-5.56	107.79	121.70
1	M	126	GLY	CA-C-O	-5.56	110.59	120.60
1	C	327	PHE	CA-C-O	5.56	131.77	120.10
1	G	93	PHE	CB-CA-C	-5.56	99.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	ALA	CA-C-N	5.56	129.43	117.20
1	A	359	ALA	C-N-CA	5.56	135.59	121.70
1	N	195	ASP	CB-CA-C	-5.56	99.28	110.40
1	J	345	THR	CA-C-O	5.56	131.77	120.10
1	K	107	LYS	CD-CE-NZ	5.56	124.48	111.70
1	F	325	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	P	1	ALA	CA-C-O	5.55	131.76	120.10
1	F	155	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	H	98	LYS	CA-CB-CG	5.55	125.61	113.40
1	H	158	PRO	O-C-N	5.55	131.58	122.70
1	I	315	GLY	CA-C-O	-5.55	110.61	120.60
1	O	65	VAL	CA-CB-CG2	5.55	119.23	110.90
1	O	36	VAL	O-C-N	5.55	132.63	123.20
1	N	203	TYR	CB-CG-CD2	5.55	124.33	121.00
1	A	154	ALA	CB-CA-C	-5.55	101.78	110.10
1	A	336	GLN	CA-CB-CG	5.55	125.60	113.40
1	B	243	TYR	CZ-CE2-CD2	5.55	124.79	119.80
1	P	261	PRO	O-C-N	-5.55	113.83	122.70
1	B	231	ASN	CA-C-N	-5.54	105.00	117.20
1	Q	171	ALA	N-CA-CB	5.54	117.86	110.10
1	P	54	ASN	O-C-N	5.54	131.57	122.70
1	I	42	ARG	NH1-CZ-NH2	-5.54	113.30	119.40
1	K	221	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	P	149	ALA	N-CA-CB	5.54	117.86	110.10
1	F	169	ALA	N-CA-CB	5.54	117.86	110.10
1	D	1	ALA	N-CA-C	5.54	125.95	111.00
1	K	23	VAL	C-N-CA	5.54	135.54	121.70
1	K	195	ASP	CA-CB-CG	-5.54	101.22	113.40
1	E	330	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	203	TYR	N-CA-CB	-5.54	100.64	110.60
1	E	293	LYS	CB-CG-CD	-5.54	97.21	111.60
1	G	66	ASP	CB-CG-OD1	5.54	123.28	118.30
1	P	52	GLU	CG-CD-OE1	5.54	129.37	118.30
1	P	327	PHE	CA-C-O	5.54	131.73	120.10
1	H	128	ASP	O-C-N	-5.53	113.80	123.20
1	M	143	ASP	CA-C-N	5.53	129.37	117.20
1	B	154	ALA	CA-C-O	-5.53	108.48	120.10
1	E	163	ILE	O-C-N	-5.53	113.85	122.70
1	I	10	GLU	CB-CA-C	-5.53	99.34	110.40
1	R	342	TYR	O-C-N	5.53	131.55	122.70
1	P	137	TYR	CG-CD2-CE2	-5.53	116.88	121.30
1	B	344	HIS	CB-CA-C	5.53	121.46	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	154	ALA	CB-CA-C	-5.53	101.81	110.10
1	N	330	ARG	CG-CD-NE	5.53	123.41	111.80
1	G	10	GLU	CA-C-O	-5.52	108.50	120.10
1	I	317	ALA	O-C-N	5.52	131.54	122.70
1	N	78	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	O	136	GLN	O-C-N	-5.52	113.86	122.70
1	K	19	ALA	CB-CA-C	5.52	118.39	110.10
1	F	109	ASP	OD1-CG-OD2	5.52	133.79	123.30
1	I	213	TYR	C-N-CA	-5.52	107.90	121.70
1	B	33	ASP	CA-C-O	-5.52	108.51	120.10
1	G	194	GLY	CA-C-O	5.52	130.53	120.60
1	G	4	PHE	CB-CA-C	-5.52	99.37	110.40
1	Q	171	ALA	CB-CA-C	-5.52	101.82	110.10
1	N	190	VAL	O-C-N	-5.52	113.87	122.70
1	D	337	ALA	N-CA-CB	5.51	117.82	110.10
1	J	160	SER	C-N-CA	-5.51	107.92	121.70
1	M	2	HIS	CA-C-N	5.51	129.33	117.20
1	Q	137	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	G	7	LEU	CA-CB-CG	5.51	127.97	115.30
1	Q	296	LYS	CB-CA-C	-5.51	99.38	110.40
1	D	123	THR	CB-CA-C	-5.51	96.73	111.60
1	K	123	THR	N-CA-CB	5.51	120.77	110.30
1	F	172	ARG	N-CA-CB	5.51	120.51	110.60
1	M	29	ILE	CB-CG1-CD1	-5.51	98.48	113.90
1	N	81	GLU	CB-CG-CD	5.51	129.07	114.20
1	N	341	GLN	C-N-CA	-5.51	107.94	121.70
1	O	338	ALA	CB-CA-C	-5.51	101.84	110.10
1	H	133	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	M	156	GLN	CG-CD-OE1	-5.50	110.59	121.60
1	B	303	ARG	CG-CD-NE	5.50	123.36	111.80
1	M	272	GLY	C-N-CA	-5.50	110.74	122.30
1	C	243	TYR	CG-CD2-CE2	-5.50	116.90	121.30
1	I	113	ALA	N-CA-CB	5.50	117.80	110.10
1	Q	89	GLN	N-CA-C	-5.50	96.15	111.00
1	R	215	ALA	CB-CA-C	-5.50	101.85	110.10
1	P	116	ALA	N-CA-CB	-5.50	102.40	110.10
1	G	168	ASN	CA-CB-CG	-5.50	101.30	113.40
1	C	174	ALA	N-CA-CB	5.50	117.80	110.10
1	G	260	VAL	CG1-CB-CG2	5.50	119.69	110.90
1	F	152	ARG	CA-C-N	-5.49	105.11	117.20
1	O	115	LEU	CA-CB-CG	5.49	127.94	115.30
1	O	267	ILE	CG1-CB-CG2	-5.49	99.31	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	328	MET	CA-CB-CG	-5.49	103.96	113.30
1	A	281	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	F	5	PRO	C-N-CA	-5.49	107.97	121.70
1	F	56	ARG	CA-CB-CG	5.49	125.48	113.40
1	K	14	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	M	36	VAL	C-N-CA	-5.49	110.77	122.30
1	F	133	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	M	225	GLY	CA-C-N	-5.49	105.13	117.20
1	B	301	TYR	CZ-CE2-CD2	5.49	124.74	119.80
1	E	332	MET	CA-C-O	5.49	131.62	120.10
1	I	165	GLU	CB-CG-CD	-5.49	99.39	114.20
1	K	4	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	P	9	GLN	C-N-CA	-5.49	107.98	121.70
1	A	324	GLN	O-C-N	-5.48	113.93	122.70
1	C	218	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	K	9	GLN	C-N-CA	-5.48	107.99	121.70
1	K	189	GLU	CG-CD-OE1	5.48	129.27	118.30
1	P	24	ALA	C-N-CA	-5.48	107.99	121.70
1	Q	32	ALA	N-CA-CB	-5.48	102.42	110.10
1	E	243	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	M	90	GLY	O-C-N	5.48	131.47	122.70
1	P	165	GLU	CB-CA-C	5.48	121.36	110.40
1	B	243	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	K	287	ASN	CB-CG-ND2	-5.47	103.56	116.70
1	N	179	GLN	CG-CD-NE2	-5.47	103.56	116.70
1	O	258	ARG	CA-CB-CG	5.47	125.44	113.40
1	C	10	GLU	N-CA-CB	5.47	120.45	110.60
1	Q	38	THR	N-CA-CB	-5.47	99.91	110.30
1	R	220	HIS	O-C-N	-5.47	113.95	122.70
1	B	301	TYR	CG-CD2-CE2	-5.47	116.92	121.30
1	O	109	ASP	CA-C-O	5.47	131.59	120.10
1	B	8	THR	CA-CB-CG2	-5.47	104.75	112.40
1	G	115	LEU	CA-CB-CG	5.47	127.87	115.30
1	J	219	HIS	CA-CB-CG	5.47	122.89	113.60
1	K	95	ASN	N-CA-CB	5.47	120.44	110.60
1	G	332	MET	CG-SD-CE	-5.46	91.46	100.20
1	K	235	ALA	N-CA-CB	5.46	117.75	110.10
1	B	91	LYS	CA-CB-CG	-5.46	101.38	113.40
1	G	66	ASP	CA-C-N	-5.46	105.18	117.20
1	B	78	LEU	O-C-N	5.46	131.44	122.70
1	B	148	ARG	CB-CA-C	-5.46	99.48	110.40
1	B	201	CYS	O-C-N	-5.46	113.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	212	VAL	CA-C-O	5.46	131.57	120.10
1	L	140	ASP	CB-CG-OD2	5.46	123.22	118.30
1	O	90	GLY	CA-C-O	-5.46	110.77	120.60
1	K	132	GLU	O-C-N	5.46	131.44	122.70
1	A	202	GLN	CB-CG-CD	-5.46	97.41	111.60
1	L	66	ASP	O-C-N	-5.46	113.97	122.70
1	L	84	TYR	CZ-CE2-CD2	-5.46	114.89	119.80
1	O	79	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	Q	168	ASN	CB-CG-ND2	-5.46	103.61	116.70
1	E	265	PRO	C-N-CA	-5.45	110.85	122.30
1	B	181	GLY	CA-C-O	-5.45	110.79	120.60
1	I	186	VAL	O-C-N	-5.45	113.98	122.70
1	J	211	ALA	O-C-N	-5.45	113.98	122.70
1	P	214	LYS	O-C-N	5.45	131.42	122.70
1	R	134	CYS	O-C-N	-5.45	113.98	122.70
1	B	123	THR	N-CA-CB	5.45	120.66	110.30
1	G	124	ILE	C-N-CA	5.45	135.33	121.70
1	L	62	LEU	CB-CG-CD2	5.45	120.27	111.00
1	A	123	THR	N-CA-CB	5.45	120.65	110.30
1	D	327	PHE	CD1-CE1-CZ	-5.45	113.56	120.10
1	B	3	ARG	N-CA-CB	5.45	120.41	110.60
1	Q	12	LYS	CB-CG-CD	-5.45	97.44	111.60
1	A	45	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	G	339	LYS	CA-CB-CG	5.44	125.38	113.40
1	I	24	ALA	N-CA-CB	5.44	117.72	110.10
1	N	305	LEU	N-CA-CB	5.44	121.28	110.40
1	P	154	ALA	N-CA-CB	-5.44	102.48	110.10
1	B	89	GLN	N-CA-C	-5.44	96.31	111.00
1	J	191	ILE	CB-CG1-CD1	-5.44	98.67	113.90
1	D	3	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	P	27	LYS	CA-CB-CG	-5.43	101.44	113.40
1	R	264	VAL	CG1-CB-CG2	-5.43	102.20	110.90
1	E	162	ALA	CB-CA-C	-5.43	101.95	110.10
1	G	191	ILE	CG1-CB-CG2	-5.43	99.45	111.40
1	I	206	GLU	CG-CD-OE2	5.43	129.17	118.30
1	C	98	LYS	CD-CE-NZ	5.43	124.19	111.70
1	J	342	TYR	CB-CG-CD1	5.43	124.26	121.00
1	A	199	GLU	CG-CD-OE1	5.43	129.16	118.30
1	D	258	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
1	H	179	GLN	O-C-N	-5.43	114.01	122.70
1	B	215	ALA	N-CA-C	5.43	125.66	111.00
1	I	66	ASP	C-N-CA	5.43	135.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	GLN	CB-CA-C	5.43	121.25	110.40
1	D	152	ARG	CA-C-O	-5.43	108.71	120.10
1	F	199	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	H	9	GLN	O-C-N	5.43	131.38	122.70
1	Q	6	ALA	O-C-N	5.43	131.38	122.70
1	R	194	GLY	CA-C-O	5.43	130.37	120.60
1	D	100	LYS	CD-CE-NZ	5.42	124.18	111.70
1	E	139	LYS	N-CA-CB	5.42	120.36	110.60
1	B	269	PHE	CD1-CG-CD2	-5.42	111.25	118.30
1	F	164	GLN	O-C-N	-5.42	114.03	122.70
1	M	26	GLY	CA-C-O	-5.42	110.84	120.60
1	D	87	ASP	OD1-CG-OD2	5.42	133.59	123.30
1	E	81	GLU	CA-CB-CG	5.42	125.32	113.40
1	I	130	LEU	CA-C-O	5.42	131.48	120.10
1	L	25	ASN	N-CA-CB	5.42	120.36	110.60
1	R	267	ILE	CG1-CB-CG2	-5.42	99.48	111.40
1	F	67	SER	N-CA-CB	-5.42	102.38	110.50
1	H	160	SER	O-C-N	5.42	131.37	122.70
1	M	244	THR	OG1-CB-CG2	-5.42	97.54	110.00
1	N	298	SER	N-CA-CB	-5.42	102.38	110.50
1	O	48	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	I	10	GLU	N-CA-CB	5.41	120.35	110.60
1	I	164	GLN	CB-CG-CD	5.41	125.67	111.60
1	I	329	LYS	CG-CD-CE	5.41	128.14	111.90
1	R	100	LYS	CD-CE-NZ	5.41	124.15	111.70
1	A	2	HIS	CA-CB-CG	5.41	122.80	113.60
1	C	161	LEU	CB-CG-CD2	5.41	120.19	111.00
1	H	82	THR	CA-CB-OG1	-5.41	97.64	109.00
1	I	111	GLY	CA-C-N	-5.41	105.38	116.20
1	I	272	GLY	C-N-CA	-5.41	110.94	122.30
1	J	70	ASN	CB-CG-OD1	5.41	132.42	121.60
1	R	258	ARG	CA-CB-CG	5.41	125.30	113.40
1	A	94	ARG	CA-CB-CG	-5.41	101.50	113.40
1	D	137	TYR	CG-CD2-CE2	5.41	125.63	121.30
1	I	285	ALA	N-CA-CB	5.41	117.67	110.10
1	P	143	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	N	109	ASP	CB-CG-OD2	5.40	123.16	118.30
1	R	118	THR	CA-C-N	5.40	129.09	117.20
1	G	159	SER	N-CA-CB	-5.40	102.40	110.50
1	L	191	ILE	CA-CB-CG2	5.40	121.70	110.90
1	C	45	ARG	CD-NE-CZ	5.40	131.16	123.60
1	I	298	SER	N-CA-CB	-5.40	102.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	7	LEU	CB-CA-C	-5.40	99.94	110.20
1	H	344	HIS	N-CA-C	5.40	125.58	111.00
1	N	81	GLU	CA-CB-CG	5.40	125.28	113.40
1	I	195	ASP	OD1-CG-OD2	5.40	133.56	123.30
1	J	94	ARG	CB-CA-C	-5.40	99.61	110.40
1	M	22	ILE	O-C-N	-5.40	114.06	122.70
1	H	329	LYS	CB-CG-CD	5.40	125.63	111.60
1	B	76	VAL	O-C-N	5.39	131.33	122.70
1	C	115	LEU	CB-CG-CD1	5.39	120.17	111.00
1	O	178	GLN	CA-CB-CG	-5.39	101.53	113.40
1	I	219	HIS	O-C-N	-5.39	114.07	122.70
1	I	258	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	Q	161	LEU	CB-CA-C	5.39	120.44	110.20
1	A	353	THR	CA-CB-CG2	-5.39	104.85	112.40
1	E	328	MET	CG-SD-CE	-5.39	91.57	100.20
1	C	228	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	F	5	PRO	N-CD-CG	-5.39	95.12	103.20
1	G	272	GLY	C-N-CA	-5.39	110.98	122.30
1	O	186	VAL	N-CA-CB	-5.39	99.64	111.50
1	P	148	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
1	B	202	GLN	CA-C-O	5.39	131.41	120.10
1	K	213	TYR	CZ-CE2-CD2	-5.39	114.95	119.80
1	N	296	LYS	N-CA-CB	5.39	120.30	110.60
1	D	212	VAL	O-C-N	-5.38	114.08	122.70
1	E	166	ASN	N-CA-CB	5.38	120.29	110.60
1	G	41	ASN	CA-C-O	-5.38	108.79	120.10
1	A	193	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	136	GLN	CB-CA-C	5.38	121.16	110.40
1	D	159	SER	N-CA-CB	5.38	118.57	110.50
1	L	98	LYS	CB-CA-C	-5.38	99.64	110.40
1	R	193	ASP	CB-CG-OD1	5.38	123.14	118.30
1	R	207	LYS	CG-CD-CE	5.38	128.05	111.90
1	H	151	LEU	CB-CG-CD1	5.38	120.15	111.00
1	J	114	PRO	CA-C-N	5.38	129.04	117.20
1	A	296	LYS	O-C-N	5.38	131.30	122.70
1	N	148	ARG	O-C-N	5.38	131.30	122.70
1	P	193	ASP	OD1-CG-OD2	-5.38	113.08	123.30
1	Q	100	LYS	CB-CA-C	-5.38	99.65	110.40
1	H	162	ALA	C-N-CA	-5.38	108.26	121.70
1	A	60	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	B	23	VAL	N-CA-C	-5.37	96.49	111.00
1	I	300	SER	N-CA-C	-5.37	96.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	23	VAL	CA-CB-CG1	5.37	118.96	110.90
1	G	2	HIS	CA-C-N	5.37	129.01	117.20
1	N	180	ASN	N-CA-CB	-5.37	100.94	110.60
1	I	215	ALA	CA-C-O	-5.37	108.83	120.10
1	I	243	TYR	CB-CG-CD1	5.37	124.22	121.00
1	M	70	ASN	O-C-N	5.37	131.29	122.70
1	N	194	GLY	C-N-CA	5.37	135.12	121.70
1	F	123	THR	CA-CB-OG1	5.37	120.27	109.00
1	J	3	ARG	CB-CG-CD	5.37	125.55	111.60
1	J	296	LYS	CD-CE-NZ	5.37	124.04	111.70
1	N	221	VAL	CA-C-N	5.37	129.00	117.20
1	P	60	GLU	O-C-N	5.37	131.28	122.70
1	Q	210	ALA	CA-C-O	-5.37	108.83	120.10
1	L	95	ASN	CA-CB-CG	-5.36	101.60	113.40
1	H	2	HIS	O-C-N	-5.36	114.12	122.70
1	F	26	GLY	C-N-CA	-5.36	108.30	121.70
1	M	126	GLY	O-C-N	5.36	131.28	122.70
1	O	30	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	A	119	ASN	CA-C-O	-5.36	108.85	120.10
1	E	149	ALA	O-C-N	5.36	131.28	122.70
1	N	243	TYR	CZ-CE2-CD2	5.36	124.62	119.80
1	R	165	GLU	N-CA-CB	-5.36	100.95	110.60
1	O	95	ASN	CA-CB-CG	-5.36	101.61	113.40
1	R	31	ALA	O-C-N	5.36	131.27	122.70
1	R	147	TRP	CZ3-CH2-CZ2	-5.36	115.17	121.60
1	C	11	GLN	O-C-N	5.36	131.27	122.70
1	O	332	MET	CA-CB-CG	-5.36	104.20	113.30
1	B	7	LEU	CD1-CG-CD2	-5.35	94.44	110.50
1	B	345	THR	N-CA-C	-5.35	96.54	111.00
1	D	24	ALA	CB-CA-C	-5.35	102.07	110.10
1	C	65	VAL	N-CA-CB	-5.35	99.73	111.50
1	G	133	ARG	CD-NE-CZ	5.35	131.09	123.60
1	H	231	ASN	CB-CG-OD1	-5.35	110.90	121.60
1	N	140	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	C	11	GLN	C-N-CA	-5.35	108.33	121.70
1	H	330	ARG	CD-NE-CZ	5.35	131.09	123.60
1	M	100	LYS	CA-CB-CG	5.35	125.16	113.40
1	Q	29	ILE	N-CA-CB	-5.35	98.50	110.80
1	Q	118	THR	N-CA-CB	-5.35	100.14	110.30
1	O	300	SER	N-CA-C	-5.35	96.57	111.00
1	B	89	GLN	CB-CG-CD	-5.34	97.70	111.60
1	D	91	LYS	N-CA-C	-5.34	96.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	336	GLN	O-C-N	5.34	131.25	122.70
1	N	110	GLN	CA-CB-CG	-5.34	101.64	113.40
1	F	279	ALA	N-CA-CB	5.34	117.58	110.10
1	J	195	ASP	CA-CB-CG	-5.34	101.65	113.40
1	O	80	HIS	CA-CB-CG	-5.34	104.52	113.60
1	F	110	GLN	CA-CB-CG	5.34	125.15	113.40
1	N	16	SER	N-CA-CB	-5.34	102.49	110.50
1	J	160	SER	CB-CA-C	-5.34	99.96	110.10
1	F	269	PHE	CB-CG-CD2	5.33	124.53	120.80
1	I	152	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
1	J	117	GLY	O-C-N	5.33	131.23	122.70
1	M	55	ARG	CD-NE-CZ	5.33	131.07	123.60
1	N	194	GLY	CA-C-O	5.33	130.20	120.60
1	A	239	CYS	CA-CB-SG	-5.33	104.40	114.00
1	J	146	LYS	CB-CG-CD	-5.33	97.74	111.60
1	C	261	PRO	N-CA-CB	5.33	109.69	103.30
1	F	167	ALA	N-CA-CB	5.33	117.56	110.10
1	R	124	ILE	N-CA-CB	-5.33	98.54	110.80
1	A	238	ALA	CB-CA-C	-5.33	102.11	110.10
1	D	89	GLN	CA-C-N	5.33	126.85	116.20
1	D	92	LEU	N-CA-CB	-5.33	99.75	110.40
1	I	107	LYS	O-C-N	-5.33	114.18	122.70
1	L	289	CYS	CA-CB-SG	-5.33	104.41	114.00
1	L	150	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	D	119	ASN	N-CA-CB	-5.32	101.02	110.60
1	G	156	GLN	CG-CD-OE1	-5.32	110.95	121.60
1	L	295	TRP	CB-CG-CD2	5.32	133.52	126.60
1	A	25	ASN	N-CA-CB	5.32	120.17	110.60
1	B	180	ASN	O-C-N	-5.32	114.15	123.20
1	G	20	GLN	N-CA-CB	-5.32	101.03	110.60
1	N	115	LEU	O-C-N	-5.32	114.19	122.70
1	Q	60	GLU	CG-CD-OE2	5.32	128.94	118.30
1	A	119	ASN	C-N-CA	5.32	134.99	121.70
1	A	358	THR	N-CA-C	-5.32	96.64	111.00
1	D	71	GLN	O-C-N	5.32	131.21	122.70
1	H	3	ARG	CB-CG-CD	5.32	125.43	111.60
1	I	60	GLU	O-C-N	-5.32	114.19	122.70
1	R	62	LEU	CB-CG-CD1	5.32	120.04	111.00
1	N	154	ALA	O-C-N	5.32	131.21	122.70
1	O	89	GLN	O-C-N	-5.32	114.16	123.20
1	B	344	HIS	N-CA-C	-5.31	96.65	111.00
1	L	151	LEU	CB-CG-CD1	5.31	120.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	213	TYR	CA-CB-CG	-5.31	103.30	113.40
1	B	22	ILE	C-N-CA	-5.31	108.42	121.70
1	B	186	VAL	N-CA-CB	-5.31	99.81	111.50
1	N	113	ALA	CB-CA-C	5.31	118.07	110.10
1	R	74	GLY	C-N-CA	-5.31	111.14	122.30
1	B	183	VAL	O-C-N	5.31	131.19	121.10
1	E	82	THR	CA-CB-CG2	-5.31	104.97	112.40
1	M	152	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	D	307	ALA	O-C-N	-5.31	114.20	122.70
1	N	167	ALA	C-N-CA	-5.31	108.42	121.70
1	R	312	ALA	O-C-N	-5.31	114.21	122.70
1	B	21	SER	CA-C-O	-5.31	108.95	120.10
1	F	342	TYR	CB-CG-CD1	5.31	124.18	121.00
1	J	42	ARG	CG-CD-NE	5.31	122.95	111.80
1	J	123	THR	CB-CA-C	-5.31	97.27	111.60
1	N	244	THR	OG1-CB-CG2	-5.31	97.79	110.00
1	F	345	THR	CB-CA-C	5.31	125.92	111.60
1	F	353	THR	N-CA-CB	-5.31	100.22	110.30
1	C	109	ASP	N-CA-CB	5.30	120.15	110.60
1	D	193	ASP	CB-CA-C	-5.30	99.79	110.40
1	G	328	MET	CA-CB-CG	5.30	122.32	113.30
1	I	305	LEU	C-N-CA	-5.30	108.44	121.70
1	H	149	ALA	C-N-CA	-5.30	108.45	121.70
1	I	115	LEU	N-CA-CB	-5.30	99.80	110.40
1	L	9	GLN	CA-CB-CG	-5.30	101.74	113.40
1	I	24	ALA	CA-C-O	-5.30	108.97	120.10
1	J	141	GLY	O-C-N	-5.30	114.22	122.70
1	Q	125	GLN	CG-CD-NE2	5.30	129.42	116.70
1	C	121	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	I	312	ALA	CB-CA-C	-5.30	102.15	110.10
1	J	328	MET	CA-CB-CG	-5.30	104.29	113.30
1	A	123	THR	CB-CA-C	-5.30	97.30	111.60
1	B	343	VAL	CA-C-N	-5.30	105.55	117.20
1	D	291	LEU	CA-CB-CG	5.30	127.48	115.30
1	E	1	ALA	N-CA-C	5.30	125.30	111.00
1	I	78	LEU	CB-CG-CD2	-5.30	102.00	111.00
1	I	187	GLU	CG-CD-OE2	5.30	128.89	118.30
1	K	99	GLU	O-C-N	5.30	131.18	122.70
1	M	236	GLY	CA-C-O	5.30	130.13	120.60
1	Q	170	LEU	O-C-N	-5.30	114.22	122.70
1	R	178	GLN	N-CA-CB	5.30	120.13	110.60
1	L	343	VAL	CB-CA-C	5.29	121.46	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	LEU	CB-CG-CD1	5.29	120.00	111.00
1	I	68	SER	CB-CA-C	-5.29	100.05	110.10
1	I	222	TYR	CB-CG-CD2	5.29	124.17	121.00
1	N	188	PRO	CA-C-N	5.29	128.84	117.20
1	O	90	GLY	C-N-CA	-5.29	108.47	121.70
1	C	195	ASP	CA-CB-CG	-5.29	101.77	113.40
1	L	322	ALA	N-CA-CB	5.29	117.50	110.10
1	Q	168	ASN	CB-CG-OD1	5.29	132.18	121.60
1	A	157	CYS	CA-CB-SG	-5.29	104.49	114.00
1	E	13	LYS	O-C-N	-5.28	114.25	122.70
1	E	182	LEU	CA-C-O	-5.28	109.01	120.10
1	D	261	PRO	CA-C-O	5.28	132.87	120.20
1	K	205	THR	C-N-CA	-5.28	108.50	121.70
1	C	39	MET	CG-SD-CE	-5.28	91.75	100.20
1	K	83	LEU	O-C-N	5.28	131.15	122.70
1	O	190	VAL	CA-CB-CG1	-5.28	102.98	110.90
1	D	341	GLN	CG-CD-OE1	5.28	132.15	121.60
1	F	34	GLU	CG-CD-OE2	-5.28	107.75	118.30
1	H	334	ASN	O-C-N	-5.28	114.26	122.70
1	M	25	ASN	N-CA-C	-5.28	96.75	111.00
1	P	172	ARG	NH1-CZ-NH2	5.28	125.20	119.40
1	I	206	GLU	C-N-CA	-5.27	108.52	121.70
1	L	180	ASN	CB-CG-OD1	-5.27	111.06	121.60
1	R	52	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	D	27	LYS	CD-CE-NZ	5.27	123.82	111.70
1	K	224	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	A	148	ARG	CA-C-O	-5.27	109.04	120.10
1	C	199	GLU	CB-CG-CD	5.27	128.42	114.20
1	G	9	GLN	OE1-CD-NE2	-5.27	109.79	121.90
1	M	137	TYR	CA-C-O	5.27	131.16	120.10
1	A	106	ILE	CG1-CB-CG2	-5.27	99.81	111.40
1	O	154	ALA	CB-CA-C	-5.27	102.20	110.10
1	I	252	THR	CA-C-N	5.26	128.78	117.20
1	K	348	SER	CA-C-O	-5.26	109.05	120.10
1	J	282	ASN	CA-C-O	-5.26	109.05	120.10
1	K	29	ILE	CG1-CB-CG2	-5.26	99.82	111.40
1	K	148	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	M	148	ARG	CD-NE-CZ	5.26	130.97	123.60
1	P	337	ALA	N-CA-CB	5.26	117.47	110.10
1	R	34	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	R	172	ARG	N-CA-CB	5.26	120.07	110.60
1	A	300	SER	N-CA-C	-5.26	96.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	94	ARG	CG-CD-NE	-5.26	100.76	111.80
1	G	94	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	I	277	GLU	O-C-N	5.26	131.12	122.70
1	P	239	CYS	CA-CB-SG	-5.26	104.53	114.00
1	P	352	SER	C-N-CA	5.26	134.85	121.70
1	K	52	GLU	CA-C-N	5.26	128.76	117.20
1	O	154	ALA	CA-C-O	-5.26	109.06	120.10
1	A	279	ALA	N-CA-CB	5.25	117.45	110.10
1	C	81	GLU	CB-CG-CD	5.25	128.38	114.20
1	H	305	LEU	O-C-N	-5.25	114.30	122.70
1	Q	198	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	M	127	LEU	O-C-N	5.25	131.10	122.70
1	H	97	LEU	C-N-CA	-5.25	108.58	121.70
1	L	172	ARG	CG-CD-NE	-5.25	100.78	111.80
1	F	279	ALA	O-C-N	-5.25	114.31	122.70
1	M	195	ASP	OD1-CG-OD2	5.25	133.27	123.30
1	C	148	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	R	27	LYS	N-CA-CB	-5.24	101.16	110.60
1	B	216	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	D	90	GLY	CA-C-O	-5.24	111.17	120.60
1	D	52	GLU	N-CA-CB	5.24	120.03	110.60
1	D	82	THR	CA-CB-CG2	-5.24	105.06	112.40
1	D	309	ALA	N-CA-CB	5.24	117.44	110.10
1	J	115	LEU	CA-CB-CG	5.24	127.35	115.30
1	M	69	ILE	N-CA-C	-5.24	96.86	111.00
1	P	343	VAL	N-CA-CB	5.24	123.02	111.50
1	B	225	GLY	O-C-N	5.24	131.08	122.70
1	J	264	VAL	CA-CB-CG2	5.24	118.75	110.90
1	E	162	ALA	N-CA-CB	5.23	117.43	110.10
1	E	258	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
1	L	186	VAL	CA-C-O	-5.23	109.11	120.10
1	Q	66	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	Q	207	LYS	CA-CB-CG	5.23	124.91	113.40
1	R	65	VAL	O-C-N	-5.23	114.33	122.70
1	B	10	GLU	CB-CA-C	-5.23	99.93	110.40
1	D	74	GLY	C-N-CA	5.23	133.29	122.30
1	F	150	VAL	CA-CB-CG1	-5.23	103.05	110.90
1	F	248	VAL	CA-C-O	5.23	131.09	120.10
1	G	68	SER	N-CA-CB	-5.23	102.65	110.50
1	H	135	ALA	CB-CA-C	-5.23	102.25	110.10
1	O	6	ALA	CB-CA-C	-5.23	102.25	110.10
1	O	236	GLY	CA-C-O	5.23	130.01	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	233	VAL	CA-CB-CG1	-5.23	103.06	110.90
1	N	241	LYS	CB-CG-CD	5.23	125.19	111.60
1	O	258	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	161	LEU	CB-CG-CD2	-5.23	102.12	111.00
1	C	169	ALA	CB-CA-C	5.23	117.94	110.10
1	H	175	SER	CB-CA-C	-5.23	100.17	110.10
1	L	38	THR	CA-C-N	-5.23	105.70	117.20
1	L	199	GLU	N-CA-CB	-5.23	101.19	110.60
1	M	24	ALA	CB-CA-C	-5.23	102.26	110.10
1	A	62	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	D	300	SER	N-CA-CB	5.22	118.34	110.50
1	G	267	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	K	134	CYS	O-C-N	-5.22	114.34	122.70
1	L	26	GLY	N-CA-C	-5.22	100.04	113.10
1	G	167	ALA	N-CA-CB	5.22	117.41	110.10
1	M	295	TRP	N-CA-CB	-5.22	101.20	110.60
1	N	56	ARG	NH1-CZ-NH2	5.22	125.15	119.40
1	D	296	LYS	N-CA-CB	5.22	120.00	110.60
1	L	229	LYS	O-C-N	5.22	131.02	121.10
1	Q	24	ALA	CA-C-N	5.22	128.69	117.20
1	B	330	ARG	CG-CD-NE	5.22	122.76	111.80
1	M	33	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	M	265	PRO	C-N-CA	-5.22	111.34	122.30
1	L	25	ASN	C-N-CA	-5.22	111.34	122.30
1	N	271	SER	N-CA-CB	-5.22	102.67	110.50
1	A	300	SER	N-CA-CB	5.22	118.32	110.50
1	C	27	LYS	N-CA-CB	-5.22	101.21	110.60
1	H	115	LEU	CA-CB-CG	5.22	127.30	115.30
1	I	257	HIS	C-N-CA	-5.22	108.66	121.70
1	Q	41	ASN	N-CA-CB	5.22	119.99	110.60
1	R	308	SER	CB-CA-C	5.22	120.01	110.10
1	C	25	ASN	C-N-CA	-5.21	111.35	122.30
1	C	276	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	M	325	GLU	CG-CD-OE2	-5.21	107.87	118.30
1	N	300	SER	N-CA-CB	5.21	118.32	110.50
1	Q	263	ALA	O-C-N	5.21	131.04	122.70
1	E	25	ASN	CA-C-N	-5.21	105.78	116.20
1	I	317	ALA	N-CA-CB	5.21	117.39	110.10
1	N	341	GLN	CA-CB-CG	-5.21	101.94	113.40
1	C	111	GLY	CA-C-N	-5.21	105.79	116.20
1	F	239	CYS	O-C-N	-5.21	114.37	122.70
1	M	3	ARG	CA-CB-CG	5.21	124.86	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	285	ALA	CB-CA-C	-5.21	102.29	110.10
1	R	114	PRO	O-C-N	5.21	131.03	122.70
1	I	206	GLU	CA-CB-CG	5.21	124.85	113.40
1	L	261	PRO	CA-C-N	-5.21	105.75	117.20
1	Q	204	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	A	338	ALA	O-C-N	5.20	131.02	122.70
1	I	217	ASN	O-C-N	5.20	131.03	122.70
1	I	232	MET	CA-CB-CG	-5.20	104.45	113.30
1	A	131	SER	N-CA-CB	-5.20	102.70	110.50
1	C	165	GLU	CB-CA-C	5.20	120.80	110.40
1	I	110	GLN	N-CA-CB	-5.20	101.24	110.60
1	E	189	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	N	180	ASN	CA-CB-CG	-5.20	101.96	113.40
1	A	248	VAL	CA-CB-CG1	5.20	118.69	110.90
1	F	258	ARG	NH1-CZ-NH2	5.20	125.11	119.40
1	M	160	SER	C-N-CA	-5.20	108.71	121.70
1	D	168	ASN	N-CA-CB	5.19	119.95	110.60
1	E	10	GLU	CA-CB-CG	5.19	124.82	113.40
1	C	88	SER	CA-CB-OG	-5.19	97.18	111.20
1	E	95	ASN	CA-CB-CG	-5.19	101.98	113.40
1	H	89	GLN	N-CA-C	-5.19	96.99	111.00
1	N	123	THR	CA-CB-OG1	-5.19	98.10	109.00
1	N	187	GLU	CG-CD-OE2	5.19	128.68	118.30
1	R	149	ALA	C-N-CA	-5.19	108.73	121.70
1	D	343	VAL	N-CA-CB	5.19	122.92	111.50
1	F	343	VAL	CB-CA-C	-5.19	101.54	111.40
1	L	266	GLY	C-N-CA	-5.19	108.73	121.70
1	N	115	LEU	CA-C-O	5.19	131.00	120.10
1	N	296	LYS	CB-CA-C	-5.19	100.02	110.40
1	G	258	ARG	CD-NE-CZ	-5.19	116.34	123.60
1	K	66	ASP	CB-CG-OD2	5.19	122.97	118.30
1	M	65	VAL	N-CA-CB	-5.19	100.09	111.50
1	Q	132	GLU	CA-CB-CG	5.19	124.81	113.40
1	G	26	GLY	C-N-CA	-5.19	108.73	121.70
1	I	69	ILE	N-CA-CB	-5.19	98.87	110.80
1	J	200	HIS	CB-CA-C	5.18	120.77	110.40
1	B	248	VAL	O-C-N	-5.18	114.41	122.70
1	J	9	GLN	O-C-N	5.18	130.99	122.70
1	K	261	PRO	O-C-N	-5.18	114.41	122.70
1	L	58	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	N	13	LYS	C-N-CA	-5.18	108.75	121.70
1	O	218	ASP	CB-CG-OD1	-5.18	113.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	LYS	CB-CA-C	-5.18	100.04	110.40
1	E	4	PHE	N-CA-CB	-5.18	101.28	110.60
1	I	180	ASN	N-CA-CB	-5.18	101.28	110.60
1	K	152	ARG	O-C-N	5.18	130.99	122.70
1	K	221	VAL	CB-CA-C	-5.18	101.56	111.40
1	A	83	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	I	26	GLY	N-CA-C	-5.18	100.15	113.10
1	A	267	ILE	CB-CG1-CD1	-5.17	99.41	113.90
1	B	326	ALA	CB-CA-C	5.17	117.86	110.10
1	G	164	GLN	CB-CG-CD	5.17	125.05	111.60
1	H	199	GLU	CA-CB-CG	5.17	124.78	113.40
1	P	123	THR	OG1-CB-CG2	5.17	121.90	110.00
1	P	250	MET	N-CA-CB	5.17	119.91	110.60
1	G	66	ASP	N-CA-C	-5.17	97.03	111.00
1	D	59	ARG	CG-CD-NE	5.17	122.66	111.80
1	G	226	THR	CA-CB-CG2	5.17	119.64	112.40
1	M	223	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	N	55	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	353	THR	CA-CB-OG1	5.17	119.85	109.00
1	D	20	GLN	CB-CA-C	-5.17	100.06	110.40
1	D	98	LYS	CB-CA-C	-5.17	100.06	110.40
1	G	250	MET	CG-SD-CE	-5.17	91.93	100.20
1	C	325	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	D	25	ASN	CA-CB-CG	5.17	124.77	113.40
1	B	272	GLY	C-N-CA	-5.17	111.45	122.30
1	D	112	GLY	C-N-CA	5.17	134.61	121.70
1	F	165	GLU	N-CA-CB	-5.17	101.30	110.60
1	A	93	PHE	CB-CG-CD1	5.16	124.42	120.80
1	B	9	GLN	CG-CD-OE1	-5.16	111.27	121.60
1	B	202	GLN	CA-CB-CG	-5.16	102.04	113.40
1	D	187	GLU	CA-CB-CG	-5.16	102.04	113.40
1	E	147	TRP	O-C-N	5.16	130.96	122.70
1	P	125	GLN	CB-CG-CD	5.16	125.03	111.60
1	A	66	ASP	CB-CG-OD1	-5.16	113.65	118.30
1	G	11	GLN	CG-CD-OE1	5.16	131.92	121.60
1	I	259	THR	O-C-N	-5.16	114.44	122.70
1	R	268	CYS	CA-CB-SG	-5.16	104.71	114.00
1	A	244	THR	N-CA-CB	-5.16	100.50	110.30
1	B	71	GLN	CG-CD-NE2	-5.16	104.32	116.70
1	G	325	GLU	CB-CG-CD	-5.16	100.27	114.20
1	K	55	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	N	297	LEU	N-CA-CB	5.16	120.72	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	228	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	F	349	GLY	N-CA-C	-5.15	100.22	113.10
1	F	350	ALA	CA-C-O	5.15	130.92	120.10
1	P	151	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	C	89	GLN	CB-CA-C	-5.15	100.10	110.40
1	L	314	GLY	C-N-CA	-5.15	111.49	122.30
1	Q	181	GLY	CA-C-O	-5.15	111.33	120.60
1	B	66	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	212	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	C	327	PHE	O-C-N	-5.15	114.46	122.70
1	P	356	LEU	CA-C-O	-5.15	109.29	120.10
1	A	124	ILE	CG1-CB-CG2	-5.15	100.08	111.40
1	M	334	ASN	CB-CA-C	5.14	120.69	110.40
1	P	258	ARG	CA-CB-CG	5.14	124.72	113.40
1	A	112	GLY	CA-C-O	5.14	129.86	120.60
1	D	97	LEU	CB-CG-CD2	5.14	119.74	111.00
1	F	266	GLY	O-C-N	5.14	130.93	122.70
1	I	93	PHE	O-C-N	-5.14	114.47	122.70
1	J	136	GLN	CG-CD-OE1	-5.14	111.32	121.60
1	K	188	PRO	N-CA-CB	5.14	109.47	103.30
1	Q	125	GLN	CG-CD-OE1	-5.14	111.32	121.60
1	Q	277	GLU	O-C-N	-5.14	114.47	122.70
1	J	279	ALA	N-CA-CB	5.14	117.30	110.10
1	B	80	HIS	CB-CA-C	-5.14	100.12	110.40
1	B	205	THR	C-N-CA	-5.14	108.85	121.70
1	J	66	ASP	CB-CG-OD2	5.14	122.93	118.30
1	J	197	ASP	OD1-CG-OD2	-5.14	113.53	123.30
1	M	175	SER	N-CA-CB	-5.14	102.79	110.50
1	R	123	THR	CA-CB-CG2	-5.14	105.21	112.40
1	K	115	LEU	CA-CB-CG	5.14	127.12	115.30
1	K	207	LYS	CD-CE-NZ	5.14	123.52	111.70
1	F	330	ARG	CB-CG-CD	5.14	124.96	111.60
1	H	329	LYS	CB-CA-C	5.14	120.67	110.40
1	Q	301	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	D	143	ASP	CA-C-O	-5.13	109.32	120.10
1	E	123	THR	N-CA-C	-5.13	97.14	111.00
1	J	166	ASN	OD1-CG-ND2	-5.13	110.09	121.90
1	Q	234	THR	O-C-N	5.13	130.92	122.70
1	E	165	GLU	CG-CD-OE1	-5.13	108.03	118.30
1	L	248	VAL	C-N-CA	-5.13	108.87	121.70
1	P	248	VAL	CA-C-O	5.13	130.88	120.10
1	H	300	SER	N-CA-C	-5.13	97.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	335	CYS	CA-CB-SG	-5.13	104.77	114.00
1	O	172	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	9	GLN	N-CA-CB	-5.13	101.37	110.60
1	C	217	ASN	OD1-CG-ND2	-5.13	110.11	121.90
1	D	336	GLN	CG-CD-OE1	5.13	131.86	121.60
1	F	109	ASP	CB-CA-C	-5.13	100.14	110.40
1	Q	225	GLY	O-C-N	5.13	130.91	122.70
1	Q	270	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	B	280	THR	C-N-CA	-5.13	108.88	121.70
1	P	105	GLY	O-C-N	-5.13	114.50	122.70
1	K	169	ALA	CB-CA-C	-5.12	102.41	110.10
1	L	77	ILE	CB-CA-C	-5.12	101.35	111.60
1	L	256	LEU	CB-CG-CD1	5.12	119.71	111.00
1	O	339	LYS	CB-CG-CD	-5.12	98.28	111.60
1	D	129	GLY	CA-C-O	5.12	129.82	120.60
1	E	123	THR	CA-CB-OG1	5.12	119.76	109.00
1	E	343	VAL	CA-C-N	5.12	128.47	117.20
1	H	147	TRP	CA-C-O	-5.12	109.34	120.10
1	P	357	PHE	C-N-CA	5.12	134.51	121.70
1	D	51	THR	O-C-N	-5.12	114.50	122.70
1	M	309	ALA	CA-C-O	5.12	130.85	120.10
1	N	124	ILE	CA-C-O	-5.12	109.35	120.10
1	H	84	TYR	CB-CG-CD1	5.12	124.07	121.00
1	G	267	ILE	C-N-CA	5.12	134.49	121.70
1	K	80	HIS	CB-CA-C	-5.12	100.17	110.40
1	O	233	VAL	CA-C-O	-5.12	109.36	120.10
1	A	147	TRP	CB-CG-CD2	5.12	133.25	126.60
1	B	344	HIS	CA-C-N	-5.12	105.94	117.20
1	I	22	ILE	CA-CB-CG2	5.12	121.13	110.90
1	O	123	THR	N-CA-CB	5.12	120.02	110.30
1	O	194	GLY	CA-C-O	5.12	129.81	120.60
1	P	60	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	Q	2	HIS	CA-CB-CG	5.12	122.30	113.60
1	Q	328	MET	CG-SD-CE	5.12	108.39	100.20
1	A	304	ALA	CA-C-O	-5.11	109.36	120.10
1	D	348	SER	CA-C-N	-5.11	105.97	116.20
1	F	291	LEU	CA-CB-CG	5.11	127.06	115.30
1	O	97	LEU	CB-CG-CD2	5.11	119.69	111.00
1	P	35	SER	CA-CB-OG	-5.11	97.40	111.20
1	B	154	ALA	O-C-N	5.11	130.88	122.70
1	B	215	ALA	O-C-N	5.11	130.88	122.70
1	D	250	MET	CG-SD-CE	-5.11	92.02	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	235	ALA	N-CA-CB	5.11	117.25	110.10
1	J	4	PHE	CZ-CE2-CD2	-5.11	113.97	120.10
1	P	318	ALA	CA-C-O	-5.11	109.38	120.10
1	R	232	MET	O-C-N	-5.11	114.53	122.70
1	B	261	PRO	CA-C-N	-5.10	105.97	117.20
1	E	88	SER	C-N-CA	5.10	134.46	121.70
1	O	140	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	53	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	L	39	MET	O-C-N	5.10	131.88	123.20
1	N	143	ASP	CA-C-O	-5.10	109.39	120.10
1	J	17	GLU	CB-CG-CD	5.10	127.97	114.20
1	B	221	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	F	352	SER	N-CA-C	5.10	124.77	111.00
1	N	305	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	D	164	GLN	OE1-CD-NE2	-5.10	110.18	121.90
1	E	167	ALA	O-C-N	5.10	130.86	122.70
1	I	221	VAL	CA-CB-CG1	-5.10	103.25	110.90
1	K	188	PRO	O-C-N	5.10	130.85	122.70
1	M	77	ILE	CB-CA-C	-5.10	101.40	111.60
1	Q	65	VAL	CA-CB-CG1	-5.10	103.25	110.90
1	A	352	SER	N-CA-CB	-5.10	102.86	110.50
1	D	109	ASP	CB-CG-OD1	5.10	122.89	118.30
1	J	161	LEU	CB-CA-C	-5.10	100.52	110.20
1	A	151	LEU	CA-CB-CG	-5.09	103.58	115.30
1	F	155	ASP	CB-CG-OD2	5.09	122.89	118.30
1	J	291	LEU	CB-CG-CD2	5.09	119.66	111.00
1	C	71	GLN	CG-CD-OE1	-5.09	111.41	121.60
1	C	206	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	K	323	THR	CA-CB-CG2	-5.09	105.27	112.40
1	A	228	LEU	O-C-N	5.09	130.85	122.70
1	E	348	SER	C-N-CA	5.09	132.99	122.30
1	L	59	ARG	CA-CB-CG	-5.09	102.20	113.40
1	L	255	ALA	N-CA-CB	-5.09	102.97	110.10
1	B	115	LEU	CA-CB-CG	5.09	127.01	115.30
1	E	18	ILE	CB-CG1-CD1	5.09	128.15	113.90
1	F	164	GLN	CB-CG-CD	5.09	124.83	111.60
1	K	119	ASN	CA-CB-CG	-5.09	102.20	113.40
1	N	139	LYS	N-CA-CB	5.09	119.76	110.60
1	O	56	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	G	179	GLN	CG-CD-NE2	-5.09	104.49	116.70
1	P	140	ASP	C-N-CA	-5.09	111.61	122.30
1	R	293	LYS	CG-CD-CE	5.09	127.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	327	PHE	CA-C-O	5.09	130.78	120.10
1	C	191	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	D	307	ALA	CB-CA-C	-5.08	102.47	110.10
1	G	72	SER	O-C-N	-5.08	114.56	122.70
1	L	59	ARG	O-C-N	5.08	130.84	122.70
1	Q	313	TRP	CE3-CZ3-CH2	-5.08	115.61	121.20
1	A	325	GLU	CB-CG-CD	-5.08	100.48	114.20
1	M	195	ASP	CA-CB-CG	-5.08	102.22	113.40
1	Q	152	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	Q	339	LYS	CA-CB-CG	5.08	124.58	113.40
1	E	190	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	O	30	LEU	O-C-N	5.08	130.83	122.70
1	G	198	LEU	CD1-CG-CD2	-5.08	95.26	110.50
1	L	218	ASP	O-C-N	5.08	130.83	122.70
1	G	110	GLN	CG-CD-NE2	-5.08	104.51	116.70
1	F	24	ALA	O-C-N	-5.08	114.58	122.70
1	L	207	LYS	CB-CA-C	5.08	120.56	110.40
1	B	168	ASN	C-N-CA	-5.08	109.01	121.70
1	N	310	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	I	191	ILE	O-C-N	-5.07	111.46	121.10
1	P	136	GLN	CA-CB-CG	-5.07	102.24	113.40
1	A	163	ILE	CA-C-O	5.07	130.75	120.10
1	A	342	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	G	334	ASN	CB-CG-OD1	-5.07	111.45	121.60
1	I	70	ASN	CA-C-N	-5.07	106.04	117.20
1	I	143	ASP	CB-CG-OD2	5.07	122.86	118.30
1	J	66	ASP	OD1-CG-OD2	-5.07	113.67	123.30
1	L	154	ALA	CA-C-O	-5.07	109.46	120.10
1	M	156	GLN	CA-CB-CG	-5.07	102.25	113.40
1	O	73	ILE	O-C-N	-5.07	114.59	123.20
1	C	342	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	F	29	ILE	O-C-N	-5.07	114.59	122.70
1	J	74	GLY	O-C-N	-5.07	114.59	123.20
1	K	28	GLY	CA-C-O	5.07	129.72	120.60
1	B	334	ASN	CA-C-N	5.06	128.33	117.20
1	H	334	ASN	CA-CB-CG	-5.06	102.27	113.40
1	J	276	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	M	127	LEU	CA-C-N	-5.06	106.07	117.20
1	F	219	HIS	CA-C-O	5.06	130.72	120.10
1	J	17	GLU	N-CA-CB	5.06	119.71	110.60
1	K	310	LEU	CB-CG-CD1	5.06	119.60	111.00
1	N	62	LEU	C-N-CA	-5.06	109.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLN	CA-C-O	5.06	130.72	120.10
1	B	277	GLU	C-N-CA	-5.06	109.06	121.70
1	F	149	ALA	CA-C-O	5.06	130.72	120.10
1	N	269	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	L	250	MET	CA-CB-CG	5.06	121.90	113.30
1	R	56	ARG	NH1-CZ-NH2	5.06	124.96	119.40
1	B	115	LEU	N-CA-CB	-5.05	100.29	110.40
1	E	2	HIS	O-C-N	-5.05	114.61	122.70
1	M	146	LYS	CA-CB-CG	5.05	124.52	113.40
1	D	320	LYS	O-C-N	-5.05	114.61	122.70
1	E	124	ILE	CB-CG1-CD1	5.05	128.04	113.90
1	F	344	HIS	CA-CB-CG	-5.05	105.01	113.60
1	J	148	ARG	CG-CD-NE	5.05	122.41	111.80
1	Q	299	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	R	3	ARG	O-C-N	5.05	130.78	122.70
1	B	95	ASN	CA-CB-CG	-5.05	102.29	113.40
1	C	277	GLU	O-C-N	5.05	130.78	122.70
1	D	321	GLU	CB-CG-CD	-5.05	100.56	114.20
1	I	66	ASP	CA-C-N	-5.05	106.09	117.20
1	J	248	VAL	CB-CA-C	-5.05	101.81	111.40
1	J	260	VAL	O-C-N	-5.05	111.50	121.10
1	O	262	ALA	N-CA-CB	-5.05	103.03	110.10
1	O	333	ALA	CB-CA-C	5.05	117.67	110.10
1	P	180	ASN	CB-CG-OD1	-5.05	111.50	121.60
1	B	22	ILE	CA-C-N	5.05	128.31	117.20
1	F	191	ILE	CG1-CB-CG2	-5.05	100.30	111.40
1	B	248	VAL	CA-CB-CG1	5.05	118.47	110.90
1	D	115	LEU	N-CA-CB	-5.05	100.31	110.40
1	D	271	SER	CA-CB-OG	-5.05	97.57	111.20
1	J	160	SER	CA-C-O	-5.05	109.50	120.10
1	J	254	THR	O-C-N	5.05	130.78	122.70
1	B	48	VAL	CA-CB-CG2	5.04	118.47	110.90
1	I	137	TYR	N-CA-CB	-5.04	101.52	110.60
1	K	339	LYS	CB-CG-CD	-5.04	98.48	111.60
1	F	174	ALA	CB-CA-C	5.04	117.67	110.10
1	M	129	GLY	N-CA-C	5.04	125.71	113.10
1	J	310	LEU	CA-CB-CG	5.04	126.90	115.30
1	N	90	GLY	O-C-N	5.04	130.77	122.70
1	L	338	ALA	CB-CA-C	-5.04	102.54	110.10
1	C	173	TYR	N-CA-CB	-5.04	101.53	110.60
1	H	125	GLN	CG-CD-NE2	5.04	128.79	116.70
1	L	131	SER	N-CA-CB	5.04	118.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	65	VAL	O-C-N	-5.04	114.64	122.70
1	B	333	ALA	C-N-CA	-5.04	109.11	121.70
1	E	147	TRP	CA-CB-CG	5.04	123.27	113.70
1	L	323	THR	O-C-N	-5.04	114.64	122.70
1	J	55	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	M	51	THR	CA-CB-CG2	5.04	119.45	112.40
1	A	127	LEU	C-N-CA	-5.03	109.11	121.70
1	G	218	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	I	186	VAL	N-CA-CB	-5.03	100.42	111.50
1	N	111	GLY	CA-C-O	5.03	129.66	120.60
1	D	275	SER	N-CA-CB	-5.03	102.95	110.50
1	F	132	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	O	118	THR	CA-C-N	5.03	128.27	117.20
1	G	189	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	P	152	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	279	ALA	C-N-CA	-5.03	109.13	121.70
1	E	109	ASP	CB-CA-C	-5.03	100.34	110.40
1	I	59	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	Q	240	THR	O-C-N	5.03	130.75	122.70
1	R	14	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	B	237	HIS	CA-CB-CG	-5.03	105.05	113.60
1	B	290	PRO	CA-C-N	5.03	128.26	117.20
1	J	300	SER	N-CA-CB	5.03	118.04	110.50
1	M	66	ASP	CA-C-O	-5.03	109.54	120.10
1	R	33	ASP	CA-CB-CG	-5.03	102.34	113.40
1	J	219	HIS	O-C-N	-5.03	114.66	122.70
1	L	291	LEU	N-CA-CB	-5.03	100.35	110.40
1	Q	91	LYS	CA-CB-CG	-5.03	102.35	113.40
1	D	270	LEU	CA-CB-CG	5.02	126.85	115.30
1	F	122	THR	CB-CA-C	-5.02	98.04	111.60
1	L	258	ARG	O-C-N	5.02	130.74	122.70
1	B	298	SER	CA-C-O	-5.02	109.56	120.10
1	E	156	GLN	CG-CD-OE1	-5.02	111.56	121.60
1	I	278	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	J	334	ASN	CB-CA-C	5.02	120.44	110.40
1	A	234	THR	CA-CB-CG2	-5.02	105.37	112.40
1	G	65	VAL	CA-CB-CG1	-5.02	103.37	110.90
1	K	109	ASP	CA-CB-CG	5.02	124.44	113.40
1	N	250	MET	O-C-N	5.02	130.73	122.70
1	R	344	HIS	CB-CA-C	-5.02	100.36	110.40
1	H	248	VAL	O-C-N	5.02	130.73	122.70
1	J	6	ALA	N-CA-CB	-5.02	103.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	312	ALA	N-CA-CB	5.02	117.12	110.10
1	P	24	ALA	CA-C-O	-5.02	109.56	120.10
1	E	286	ILE	O-C-N	-5.02	114.67	122.70
1	B	227	LEU	C-N-CA	-5.01	109.17	121.70
1	O	239	CYS	CB-CA-C	-5.01	100.37	110.40
1	P	89	GLN	OE1-CD-NE2	5.01	133.43	121.90
1	D	70	ASN	CA-C-O	-5.01	109.58	120.10
1	D	295	TRP	CB-CG-CD2	5.01	133.12	126.60
1	G	249	ALA	O-C-N	-5.01	114.68	122.70
1	M	4	PHE	N-CA-CB	-5.01	101.58	110.60
1	B	38	THR	CA-CB-CG2	-5.01	105.39	112.40
1	C	26	GLY	C-N-CA	-5.01	109.17	121.70
1	K	348	SER	N-CA-C	5.01	124.53	111.00
1	N	178	GLN	N-CA-CB	5.01	119.62	110.60
1	A	87	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	J	239	CYS	O-C-N	5.01	130.71	122.70
1	F	334	ASN	CB-CG-OD1	-5.01	111.59	121.60
1	H	191	ILE	CG1-CB-CG2	-5.01	100.39	111.40
1	R	6	ALA	O-C-N	5.01	130.71	122.70
1	R	306	GLN	N-CA-CB	-5.01	101.59	110.60
1	E	20	GLN	CA-CB-CG	-5.00	102.39	113.40
1	G	108	LEU	CB-CG-CD2	-5.00	102.49	111.00
1	O	160	SER	C-N-CA	-5.00	109.19	121.70
1	R	243	TYR	CB-CG-CD1	-5.00	118.00	121.00
1	B	14	GLU	C-N-CA	-5.00	109.19	121.70
1	G	207	LYS	CA-CB-CG	5.00	124.41	113.40
1	J	87	ASP	CB-CG-OD1	-5.00	113.80	118.30
1	L	186	VAL	N-CA-CB	-5.00	100.49	111.50
1	N	258	ARG	N-CA-CB	5.00	119.61	110.60
1	C	168	ASN	CA-CB-CG	-5.00	102.40	113.40
1	D	319	ASN	N-CA-CB	-5.00	101.60	110.60
1	F	54	ASN	CB-CG-OD1	-5.00	111.60	121.60
1	I	203	TYR	CB-CG-CD1	-5.00	118.00	121.00
1	I	260	VAL	N-CA-CB	-5.00	100.50	111.50
1	M	65	VAL	CG1-CB-CG2	-5.00	102.90	110.90

There are no chirality outliers.

All (133) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	THR	Mainchain
1	A	153	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	159	SER	Mainchain
1	A	220	HIS	Mainchain
1	A	300	SER	Mainchain
1	A	356	LEU	Peptide
1	A	4	PHE	Mainchain
1	B	214	LYS	Mainchain
1	B	226	THR	Mainchain
1	B	248	VAL	Mainchain
1	B	267	ILE	Mainchain
1	B	292	PRO	Mainchain
1	B	300	SER	Mainchain
1	B	323	THR	Mainchain
1	B	334	ASN	Mainchain
1	B	341	GLN	Mainchain
1	B	345	THR	Mainchain
1	B	6	ALA	Mainchain
1	B	68	SER	Mainchain
1	B	69	ILE	Mainchain
1	C	115	LEU	Mainchain
1	C	263	ALA	Mainchain
1	C	296	LYS	Mainchain
1	C	300	SER	Mainchain
1	C	35	SER	Mainchain
1	C	87	ASP	Mainchain
1	D	1	ALA	Peptide
1	D	100	LYS	Mainchain
1	D	159	SER	Mainchain
1	D	18	ILE	Mainchain
1	D	195	ASP	Mainchain
1	D	226	THR	Mainchain
1	D	24	ALA	Mainchain
1	D	285	ALA	Mainchain
1	D	306	GLN	Mainchain
1	D	33	ASP	Mainchain
1	D	70	ASN	Mainchain
1	D	87	ASP	Mainchain
1	D	89	GLN	Mainchain
1	E	100	LYS	Mainchain
1	E	123	THR	Mainchain
1	E	196	HIS	Mainchain
1	E	247	GLN	Mainchain
1	E	258	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	E	88	SER	Mainchain,Peptide
1	F	190	VAL	Mainchain
1	F	26	GLY	Mainchain
1	F	319	ASN	Mainchain
1	F	70	ASN	Mainchain
1	G	113	ALA	Mainchain
1	G	229	LYS	Mainchain
1	G	3	ARG	Mainchain
1	G	300	SER	Mainchain
1	G	65	VAL	Mainchain
1	G	83	LEU	Mainchain
1	G	87	ASP	Mainchain
1	G	98	LYS	Mainchain
1	H	1	ALA	Peptide
1	H	166	ASN	Mainchain
1	H	3	ARG	Mainchain
1	H	300	SER	Mainchain
1	H	345	THR	Mainchain
1	H	70	ASN	Mainchain
1	H	89	GLN	Mainchain
1	I	109	ASP	Mainchain
1	I	115	LEU	Mainchain
1	I	148	ARG	Mainchain
1	I	154	ALA	Mainchain
1	I	176	ILE	Mainchain
1	I	204	VAL	Mainchain
1	I	331	ALA	Mainchain
1	I	338	ALA	Mainchain
1	I	66	ASP	Peptide
1	I	67	SER	Mainchain
1	I	69	ILE	Mainchain
1	J	108	LEU	Mainchain
1	J	24	ALA	Mainchain
1	J	33	ASP	Mainchain
1	J	70	ASN	Mainchain
1	K	189	GLU	Mainchain
1	K	300	SER	Mainchain
1	K	347	SER	Mainchain,Peptide
1	K	4	PHE	Mainchain
1	K	88	SER	Mainchain
1	L	12	LYS	Mainchain
1	L	180	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	L	296	LYS	Mainchain
1	L	333	ALA	Mainchain
1	L	338	ALA	Mainchain
1	L	87	ASP	Mainchain
1	M	282	ASN	Mainchain
1	M	344	HIS	Mainchain
1	M	352	SER	Peptide
1	M	356	LEU	Mainchain
1	M	358	THR	Mainchain
1	M	68	SER	Mainchain
1	M	69	ILE	Peptide
1	M	71	GLN	Mainchain
1	N	109	ASP	Mainchain
1	N	116	ALA	Mainchain
1	N	298	SER	Mainchain
1	N	3	ARG	Peptide
1	N	35	SER	Mainchain
1	N	87	ASP	Mainchain
1	O	116	ALA	Mainchain
1	O	180	ASN	Mainchain
1	O	267	ILE	Mainchain
1	O	297	LEU	Mainchain
1	O	300	SER	Mainchain
1	P	114	PRO	Mainchain
1	P	123	THR	Mainchain
1	P	285	ALA	Mainchain
1	P	295	TRP	Mainchain
1	P	352	SER	Mainchain
1	P	87	ASP	Mainchain
1	Q	134	CYS	Mainchain
1	Q	21	SER	Mainchain
1	Q	217	ASN	Mainchain
1	Q	300	SER	Mainchain
1	Q	87	ASP	Mainchain
1	Q	88	SER	Mainchain
1	R	113	ALA	Mainchain
1	R	134	CYS	Mainchain
1	R	161	LEU	Mainchain
1	R	171	ALA	Mainchain
1	R	220	HIS	Mainchain
1	R	237	HIS	Mainchain
1	R	266	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	R	300	SER	Mainchain
1	R	70	ASN	Mainchain
1	R	88	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2730	0	2736	243	0
1	B	2651	0	2662	264	0
1	C	2635	0	2651	219	0
1	D	2701	0	2711	217	0
1	E	2687	0	2693	194	0
1	F	2675	0	2683	168	0
1	G	2628	0	2644	153	0
1	H	2712	0	2720	209	0
1	I	2628	0	2644	256	0
1	J	2701	0	2714	195	0
1	K	2686	0	2694	151	0
1	L	2628	0	2645	191	0
1	M	2730	0	2739	251	0
1	N	2628	0	2644	234	0
1	O	2628	0	2645	209	0
1	P	2730	0	2739	177	0
1	Q	2628	0	2645	147	0
1	R	2628	0	2644	155	0
2	A	10	0	0	4	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	G	15	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	M	5	0	0	0	0
2	O	5	0	0	0	0
2	P	10	0	0	0	0
2	R	10	0	0	1	0
3	A	86	0	0	17	0
3	B	34	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	0	2	0
3	D	82	0	0	7	0
3	E	75	0	0	7	0
3	F	80	0	0	14	0
3	G	75	0	0	5	0
3	H	70	0	0	9	0
3	I	45	0	0	7	0
3	J	78	0	0	18	0
3	K	71	0	0	6	0
3	L	28	0	0	2	0
3	M	81	0	0	9	0
3	N	53	0	0	5	0
3	O	37	0	0	8	0
3	P	78	0	0	12	0
3	Q	80	0	0	10	0
3	R	72	0	0	10	0
All	All	49278	0	48253	3328	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 35.

All (3328) 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:D:70:ASN:CB	1:D:70:ASN:CA	1.74	1.64
1:D:70:ASN:HD22	1:D:70:ASN:CA	1.30	1.41
1:E:89:GLN:OE1	1:E:89:GLN:CB	1.72	1.36
1:D:70:ASN:ND2	1:D:70:ASN:CA	1.87	1.35
1:A:356:LEU:HD13	1:A:357:PHE:CE1	1.65	1.32
1:M:68:SER:CA	1:M:69:ILE:HG13	1.61	1.29
1:E:329:LYS:NZ	1:E:347:SER:HB3	1.48	1.28
1:F:69:ILE:HG22	3:F:457:HOH:O	1.24	1.28
1:M:66:ASP:O	1:M:68:SER:HA	1.34	1.23
1:M:343:VAL:HG23	1:M:344:HIS:O	1.34	1.22
1:M:69:ILE:HD13	1:M:328:MET:CE	1.69	1.22
1:A:67:SER:CB	3:A:502:HOH:O	1.87	1.21
1:D:70:ASN:C	1:D:70:ASN:CB	2.07	1.21
1:A:342:TYR:CE2	1:A:344:HIS:HB3	1.75	1.20
1:B:250:MET:HE3	1:B:291:LEU:HD21	1.26	1.18
1:J:244:THR:HG22	1:J:247:GLN:H	1.09	1.16
1:D:70:ASN:HD22	1:D:70:ASN:HA	1.02	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:51:THR:HG22	1:R:54:ASN:H	1.05	1.16
1:M:68:SER:OG	1:M:69:ILE:HD12	1.42	1.15
1:I:3:ARG:HD3	1:J:156:GLN:HE22	1.05	1.14
1:M:68:SER:O	1:M:69:ILE:C	1.78	1.14
1:N:2:HIS:HA	1:N:3:ARG:CZ	1.78	1.13
1:G:87:ASP:HB3	1:G:89:GLN:H	1.06	1.13
1:K:244:THR:HG22	1:K:247:GLN:N	1.64	1.13
1:D:70:ASN:HB3	1:D:70:ASN:O	1.49	1.12
1:M:69:ILE:CD1	1:M:328:MET:SD	2.37	1.12
1:B:342:TYR:CE2	1:B:344:HIS:HA	1.83	1.12
1:K:244:THR:CG2	1:K:247:GLN:H	1.63	1.11
1:R:244:THR:HG22	1:R:247:GLN:H	1.14	1.11
1:A:51:THR:HG22	1:A:54:ASN:H	0.99	1.11
1:P:303:ARG:HH21	1:P:357:PHE:HA	1.08	1.11
1:P:51:THR:HG22	1:P:54:ASN:H	1.03	1.11
1:A:2:HIS:HB2	1:A:3:ARG:HD2	1.31	1.11
1:L:51:THR:HG22	1:L:54:ASN:H	1.06	1.11
1:Q:119:ASN:N	1:R:1:ALA:HB1	1.65	1.10
1:H:329:LYS:HD2	1:H:347:SER:HA	1.33	1.10
1:D:88:SER:O	1:D:89:GLN:HB2	1.30	1.10
1:A:307:ALA:CB	1:A:357:PHE:HZ	1.62	1.10
1:A:45:ARG:CZ	1:A:357:PHE:HA	1.80	1.10
1:E:256:LEU:HD13	1:E:267:ILE:HD11	1.32	1.10
1:J:51:THR:HG22	1:J:54:ASN:H	1.05	1.10
1:M:329:LYS:HE3	1:M:347:SER:HB2	1.21	1.10
1:I:68:SER:HA	1:I:70:ASN:ND2	1.66	1.10
1:N:123:THR:HG22	1:N:124:ILE:H	1.07	1.09
1:C:51:THR:HG22	1:C:54:ASN:N	1.67	1.09
1:H:256:LEU:HD13	1:H:267:ILE:HD11	1.31	1.09
1:H:51:THR:HG22	1:H:54:ASN:H	0.98	1.09
1:N:256:LEU:HD13	1:N:267:ILE:HD11	1.29	1.09
1:B:51:THR:HG22	1:B:54:ASN:HB2	1.33	1.09
1:K:353:THR:HG22	3:O:509:HOH:O	1.51	1.09
1:K:51:THR:HG22	1:K:54:ASN:H	1.18	1.08
1:K:303:ARG:NH2	1:K:357:PHE:HB2	1.69	1.08
1:F:329:LYS:HE2	1:F:347:SER:HA	1.09	1.08
1:Q:51:THR:HG22	1:Q:54:ASN:H	1.07	1.08
1:M:69:ILE:HD13	1:M:328:MET:SD	1.93	1.08
1:A:244:THR:CG2	1:A:247:GLN:H	1.66	1.08
1:Q:50:ASN:ND2	1:Q:55:ARG:HH11	1.52	1.07
1:E:329:LYS:HZ2	1:E:347:SER:HB3	0.98	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:ASN:H	1:J:1:ALA:HB3	1.11	1.07
1:D:244:THR:HG22	1:D:247:GLN:H	1.18	1.07
1:H:330:ARG:HH11	1:H:347:SER:CB	1.68	1.07
1:Q:119:ASN:H	1:R:1:ALA:HB1	0.91	1.07
1:H:330:ARG:HH11	1:H:347:SER:HB2	1.18	1.06
1:P:3:ARG:HD3	1:P:4:PHE:H	1.19	1.06
1:A:307:ALA:HB2	1:A:357:PHE:CZ	1.90	1.05
1:I:68:SER:HB3	3:I:406:HOH:O	1.53	1.05
1:I:223:LEU:O	1:I:226:THR:HB	1.56	1.05
1:F:329:LYS:CE	1:F:347:SER:HA	1.86	1.05
1:A:244:THR:HG22	1:A:247:GLN:N	1.69	1.05
1:F:50:ASN:ND2	1:F:55:ARG:HH11	1.52	1.05
1:M:69:ILE:HA	1:M:71:GLN:H	1.14	1.05
1:A:307:ALA:CA	1:A:357:PHE:HZ	1.70	1.05
1:B:58:PHE:CE1	1:B:310:LEU:HD13	1.91	1.05
1:N:244:THR:HG22	1:N:247:GLN:HG3	1.38	1.04
1:M:68:SER:CA	1:M:69:ILE:CG1	2.35	1.04
1:M:69:ILE:HD13	1:M:328:MET:HE1	1.35	1.04
1:C:51:THR:CG2	1:C:54:ASN:H	1.70	1.04
1:H:352:SER:HA	1:H:354:GLN:HB2	1.39	1.04
1:I:65:VAL:HG11	1:I:69:ILE:HD13	1.39	1.04
1:B:68:SER:O	1:B:70:ASN:N	1.92	1.03
1:L:118:THR:CG2	1:L:121:GLU:H	1.71	1.03
1:N:3:ARG:CZ	1:O:203:TYR:OH	2.07	1.03
1:D:70:ASN:CG	1:D:70:ASN:CA	2.27	1.02
1:A:41:ASN:HB3	1:A:358:THR:HB	1.41	1.02
1:D:70:ASN:CB	1:D:70:ASN:O	2.06	1.02
1:E:253:VAL:HG12	1:E:291:LEU:HD23	1.40	1.02
1:O:244:THR:HG22	1:O:247:GLN:H	1.24	1.02
1:Q:119:ASN:H	1:R:1:ALA:CB	1.72	1.02
1:M:51:THR:HG22	1:M:54:ASN:H	1.25	1.02
1:D:51:THR:HG22	1:D:54:ASN:H	1.21	1.01
1:P:244:THR:HG22	1:P:247:GLN:H	1.25	1.01
1:A:244:THR:HG22	1:A:247:GLN:H	0.85	1.01
1:F:71:GLN:NE2	3:F:401:HOH:O	1.68	1.01
1:E:89:GLN:OE1	1:E:90:GLY:N	1.92	1.01
1:E:66:ASP:O	1:E:67:SER:HB3	1.58	1.01
1:I:3:ARG:HD3	1:J:156:GLN:NE2	1.75	1.00
1:B:51:THR:CG2	1:B:54:ASN:H	1.75	1.00
1:E:329:LYS:NZ	1:E:347:SER:CB	2.24	1.00
1:I:123:THR:HG22	1:I:124:ILE:H	1.24	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:THR:HG22	1:E:247:GLN:H	1.26	1.00
1:H:3:ARG:O	1:H:3:ARG:HD3	1.60	1.00
1:D:191:ILE:HD12	1:D:191:ILE:N	1.76	0.99
1:D:88:SER:O	1:D:89:GLN:CB	2.08	0.99
1:C:51:THR:HG22	1:C:54:ASN:H	0.85	0.99
1:B:51:THR:HG22	1:B:54:ASN:H	1.28	0.99
1:L:51:THR:CG2	1:L:54:ASN:H	1.75	0.99
1:Q:2:HIS:O	1:Q:3:ARG:HB2	1.63	0.99
1:E:329:LYS:HZ2	1:E:347:SER:CB	1.75	0.99
1:P:51:THR:CG2	1:P:54:ASN:H	1.76	0.99
1:A:356:LEU:HD13	1:A:357:PHE:HE1	1.20	0.99
1:L:87:ASP:HB2	1:L:91:LYS:H	1.27	0.99
1:A:50:ASN:ND2	1:A:55:ARG:HH11	1.58	0.99
1:O:51:THR:HG22	1:O:54:ASN:HB2	1.42	0.98
1:B:50:ASN:HD21	1:B:55:ARG:HD3	1.27	0.98
1:K:244:THR:HG22	1:K:247:GLN:H	0.84	0.98
1:L:87:ASP:HB3	1:L:89:GLN:H	1.25	0.98
1:I:118:THR:HA	1:J:1:ALA:N	1.77	0.98
1:A:307:ALA:HB2	1:A:357:PHE:HZ	1.25	0.98
1:L:89:GLN:HG2	1:L:89:GLN:O	1.60	0.98
1:O:3:ARG:HG2	1:O:4:PHE:H	1.28	0.98
1:P:303:ARG:HH22	1:P:357:PHE:HD1	1.09	0.97
1:J:244:THR:HB	1:J:247:GLN:HE21	1.26	0.97
1:E:12:LYS:HB3	1:E:222:TYR:CE2	2.00	0.96
1:E:250:MET:HE1	1:E:291:LEU:HD22	1.43	0.96
1:O:343:VAL:HG23	1:O:344:HIS:H	1.30	0.96
1:A:307:ALA:HA	1:A:357:PHE:CZ	2.00	0.96
1:A:307:ALA:CB	1:A:357:PHE:CZ	2.46	0.96
1:B:330:ARG:HE	1:B:330:ARG:HA	1.31	0.96
1:D:1:ALA:N	1:D:220:HIS:HE1	1.62	0.96
1:E:329:LYS:CE	1:E:347:SER:HB3	1.94	0.96
1:N:87:ASP:HB3	1:N:89:GLN:H	1.30	0.96
1:N:223:LEU:O	1:N:226:THR:HB	1.65	0.95
1:M:66:ASP:O	1:M:68:SER:N	1.99	0.95
1:A:51:THR:CG2	1:A:54:ASN:H	1.78	0.95
1:C:123:THR:HG22	1:C:124:ILE:H	1.30	0.95
1:O:156:GLN:OE1	1:P:2:HIS:HB3	1.67	0.95
1:A:51:THR:HG22	1:A:54:ASN:N	1.80	0.95
1:B:281:LEU:HD21	1:B:344:HIS:ND1	1.82	0.95
1:A:42:ARG:CD	1:A:357:PHE:HB3	1.95	0.94
1:K:303:ARG:HH21	1:K:357:PHE:HB2	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244:THR:CG2	1:L:247:GLN:H	1.79	0.94
1:Q:223:LEU:O	1:Q:226:THR:HB	1.68	0.94
1:B:203:TYR:OH	1:C:2:HIS:HA	1.67	0.94
1:M:118:THR:CG2	1:M:121:GLU:H	1.80	0.94
1:E:329:LYS:HD3	1:E:347:SER:CB	1.97	0.94
1:A:124:ILE:HD13	1:A:149:ALA:HA	1.50	0.94
1:F:67:SER:O	1:F:70:ASN:ND2	1.98	0.94
1:F:351:ALA:O	1:F:352:SER:HB2	1.66	0.94
1:M:1:ALA:HB3	1:N:119:ASN:H	1.32	0.94
1:A:207:LYS:HE2	1:D:2:HIS:NE2	1.83	0.93
1:A:67:SER:HB3	3:A:502:HOH:O	1.57	0.93
1:A:125:GLN:HE22	1:B:129:GLY:H	1.13	0.93
1:C:118:THR:CG2	1:C:121:GLU:H	1.82	0.93
1:C:87:ASP:HB3	1:C:89:GLN:H	1.33	0.93
1:H:256:LEU:HD13	1:H:267:ILE:CD1	1.99	0.93
1:A:342:TYR:HE2	1:A:344:HIS:HB3	1.31	0.93
1:D:189:GLU:HG2	1:D:191:ILE:HD12	1.51	0.93
1:P:51:THR:HG22	1:P:54:ASN:N	1.84	0.93
1:I:51:THR:HG22	1:I:53:GLU:N	1.84	0.93
1:A:115:LEU:O	1:A:118:THR:HB	1.69	0.92
1:D:189:GLU:HG2	1:D:191:ILE:CD1	1.97	0.92
1:G:119:ASN:H	1:H:1:ALA:N	1.66	0.92
1:C:159:SER:CB	1:D:1:ALA:HB3	1.98	0.92
1:E:12:LYS:HB3	1:E:222:TYR:CZ	2.04	0.92
1:N:123:THR:HG22	1:N:124:ILE:N	1.84	0.92
1:M:118:THR:HG23	1:M:121:GLU:H	1.34	0.92
1:R:124:ILE:HG22	1:R:147:TRP:CZ2	2.04	0.92
1:Q:3:ARG:HD2	1:R:156:GLN:HE22	1.33	0.92
1:G:223:LEU:O	1:G:226:THR:HB	1.70	0.92
1:R:190:VAL:H	1:R:231:ASN:ND2	1.67	0.92
1:E:329:LYS:HE2	1:E:346:GLY:O	1.70	0.92
1:H:51:THR:HG22	1:H:54:ASN:N	1.83	0.92
1:P:3:ARG:HD3	1:P:4:PHE:N	1.85	0.92
1:A:307:ALA:CA	1:A:357:PHE:CZ	2.52	0.91
1:F:71:GLN:HG3	3:F:401:HOH:O	1.69	0.91
1:A:303:ARG:HG2	1:A:357:PHE:CD1	2.05	0.91
1:K:51:THR:HG22	1:K:54:ASN:N	1.86	0.91
1:N:3:ARG:HG2	1:O:203:TYR:HE1	1.36	0.91
1:L:51:THR:HG22	1:L:54:ASN:N	1.86	0.91
1:P:303:ARG:NH2	1:P:357:PHE:HD1	1.67	0.91
1:Q:129:GLY:H	1:R:125:GLN:NE2	1.67	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:58:PHE:CZ	1:R:310:LEU:HD13	2.04	0.91
1:B:8:THR:OG1	1:B:11:GLN:HG3	1.70	0.91
1:A:207:LYS:HE2	1:D:2:HIS:CD2	2.06	0.91
1:D:87:ASP:HB2	1:D:91:LYS:H	1.32	0.91
1:D:119:ASN:O	1:D:152:ARG:NH1	2.04	0.91
1:D:58:PHE:CZ	1:D:310:LEU:HD13	2.06	0.91
1:E:2:HIS:HB3	1:F:156:GLN:OE1	1.69	0.91
1:H:330:ARG:NH1	1:H:347:SER:HB2	1.86	0.91
1:M:67:SER:O	1:M:69:ILE:HG23	1.70	0.91
1:L:50:ASN:HD21	1:L:55:ARG:HD3	1.33	0.90
1:N:313:TRP:CE2	1:N:315:GLY:HA2	2.06	0.90
1:D:1:ALA:H2	1:D:220:HIS:HE1	1.14	0.90
1:I:118:THR:HA	1:J:1:ALA:H2	1.36	0.90
1:A:223:LEU:O	1:A:226:THR:HB	1.71	0.90
1:N:3:ARG:NH1	1:O:203:TYR:CZ	2.39	0.90
1:P:291:LEU:O	1:P:293:LYS:HG3	1.72	0.90
1:R:343:VAL:O	1:R:344:HIS:ND1	2.04	0.90
1:E:250:MET:CE	1:E:291:LEU:HD22	2.00	0.90
1:Q:129:GLY:H	1:R:125:GLN:HE22	1.12	0.90
1:H:24:ALA:HA	3:H:434:HOH:O	1.70	0.90
1:I:213:TYR:OH	1:I:228:LEU:HD13	1.70	0.90
1:A:356:LEU:CD1	1:A:357:PHE:CE1	2.54	0.89
1:B:244:THR:CG2	1:B:247:GLN:H	1.85	0.89
1:B:244:THR:HG22	1:B:247:GLN:H	1.35	0.89
1:G:202:GLN:HB2	1:G:233:VAL:HG11	1.54	0.89
1:E:329:LYS:HZ3	1:E:347:SER:HA	1.36	0.89
1:H:329:LYS:CD	1:H:347:SER:HA	2.02	0.89
1:M:1:ALA:N	1:N:118:THR:HA	1.85	0.89
1:N:244:THR:CG2	1:N:247:GLN:HG3	2.01	0.89
1:B:51:THR:HG22	1:B:54:ASN:CB	2.01	0.89
1:B:61:ILE:HG21	1:B:323:THR:CG2	2.02	0.89
1:A:118:THR:HA	1:B:1:ALA:CB	2.02	0.89
1:N:3:ARG:HG2	1:O:203:TYR:CE1	2.08	0.89
1:N:51:THR:HG22	1:N:54:ASN:H	1.38	0.89
1:A:50:ASN:HD21	1:A:55:ARG:NH1	1.71	0.89
1:A:50:ASN:HD21	1:A:55:ARG:HH11	0.89	0.88
1:F:50:ASN:HD21	1:F:55:ARG:HH11	0.91	0.88
1:M:71:GLN:HG2	3:M:501:HOH:O	1.70	0.88
1:P:1:ALA:O	1:P:2:HIS:HB2	1.71	0.88
1:I:343:VAL:HG12	1:I:344:HIS:N	1.85	0.88
1:B:342:TYR:C	1:B:344:HIS:H	1.75	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:PRO:HG3	1:J:267:ILE:HD12	1.55	0.88
1:J:51:THR:HG22	1:J:54:ASN:N	1.89	0.88
1:F:69:ILE:CG2	3:F:457:HOH:O	1.95	0.88
1:A:45:ARG:HH21	1:A:358:THR:H	1.17	0.88
1:A:87:ASP:HB3	1:A:89:GLN:H	1.38	0.88
1:E:190:VAL:H	1:E:231:ASN:ND2	1.70	0.88
1:H:8:THR:HG22	1:H:10:GLU:H	1.37	0.88
1:M:69:ILE:HA	1:M:71:GLN:N	1.88	0.88
1:C:313:TRP:CE2	1:C:315:GLY:HA2	2.08	0.87
1:I:226:THR:HG23	3:I:423:HOH:O	1.74	0.87
1:M:69:ILE:HD11	1:M:328:MET:SD	2.13	0.87
2:A:401:SO4:O1	3:A:501:HOH:O	1.93	0.87
1:K:357:PHE:O	1:O:139:LYS:HE3	1.75	0.87
1:A:303:ARG:HG2	1:A:357:PHE:HD1	1.35	0.87
1:N:244:THR:HG22	1:N:247:GLN:H	1.38	0.87
1:B:344:HIS:CG	1:B:345:THR:H	1.88	0.87
1:E:125:GLN:NE2	1:F:129:GLY:H	1.72	0.87
1:P:87:ASP:HB3	1:P:89:GLN:H	1.40	0.87
1:I:68:SER:HA	1:I:70:ASN:HD22	1.33	0.87
1:I:118:THR:CA	1:J:1:ALA:N	2.36	0.87
1:Q:51:THR:HG22	1:Q:54:ASN:N	1.90	0.87
1:B:123:THR:HG23	1:B:165:GLU:HG3	1.55	0.86
1:M:69:ILE:CA	1:M:71:GLN:H	1.88	0.86
1:O:51:THR:CG2	1:O:54:ASN:H	1.88	0.86
1:E:244:THR:CG2	1:E:246:GLU:HB2	2.05	0.86
1:E:129:GLY:H	1:F:125:GLN:NE2	1.72	0.86
1:M:308:SER:HB3	1:M:351:ALA:HB1	1.55	0.86
1:M:66:ASP:O	1:M:68:SER:CA	2.23	0.86
1:N:256:LEU:HD13	1:N:267:ILE:CD1	2.05	0.86
1:H:352:SER:OG	1:H:354:GLN:HB3	1.75	0.86
1:J:8:THR:OG1	1:J:11:GLN:HG3	1.75	0.86
1:E:66:ASP:O	1:E:67:SER:CB	2.20	0.86
1:Q:1:ALA:N	3:Q:2001:HOH:O	2.08	0.86
1:O:51:THR:HG22	1:O:54:ASN:CB	2.04	0.86
1:D:1:ALA:N	1:D:220:HIS:CE1	2.42	0.86
1:B:123:THR:O	1:B:124:ILE:HD13	1.74	0.86
1:L:65:VAL:HG21	1:L:69:ILE:HG13	1.57	0.86
1:M:95:ASN:O	1:M:99:GLU:HG3	1.75	0.86
1:N:190:VAL:H	1:N:231:ASN:ND2	1.72	0.86
1:F:58:PHE:CZ	1:F:310:LEU:HD13	2.10	0.86
1:J:244:THR:HG22	1:J:247:GLN:N	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244:THR:HG23	1:L:247:GLN:H	1.40	0.86
1:A:156:GLN:OE1	1:B:2:HIS:HB3	1.75	0.86
1:A:356:LEU:O	1:A:359:ALA:HB2	1.75	0.85
1:I:129:GLY:H	1:J:125:GLN:NE2	1.73	0.85
1:I:200:HIS:HE1	1:L:2:HIS:ND1	1.74	0.85
1:M:329:LYS:CE	1:M:347:SER:HB2	2.04	0.85
1:M:345:THR:HG21	1:M:347:SER:HB3	1.57	0.85
1:Q:2:HIS:HB3	1:R:156:GLN:OE1	1.75	0.85
1:R:51:THR:HG22	1:R:54:ASN:N	1.90	0.85
1:G:156:GLN:OE1	1:H:1:ALA:HB1	1.75	0.85
1:M:1:ALA:H3	1:N:118:THR:CA	1.88	0.85
1:M:1:ALA:N	1:N:118:THR:CA	2.39	0.85
1:E:51:THR:HG22	1:E:54:ASN:H	1.40	0.85
1:H:58:PHE:CZ	1:H:310:LEU:HD13	2.12	0.85
1:J:115:LEU:O	1:J:118:THR:HB	1.76	0.85
1:A:42:ARG:HD2	1:A:357:PHE:HB3	1.59	0.85
1:D:329:LYS:NZ	1:D:347:SER:HA	1.91	0.85
1:P:303:ARG:NH2	1:P:357:PHE:HA	1.92	0.85
1:Q:156:GLN:O	1:R:1:ALA:N	2.10	0.85
1:H:352:SER:HA	1:H:354:GLN:CB	2.07	0.85
1:M:68:SER:N	1:M:69:ILE:HG13	1.91	0.85
1:Q:156:GLN:NE2	1:R:3:ARG:HE	1.73	0.85
1:G:129:GLY:H	1:H:125:GLN:NE2	1.74	0.84
1:C:213:TYR:OH	1:C:228:LEU:HD13	1.76	0.84
1:L:277:GLU:OE2	1:L:342:TYR:OH	1.95	0.84
1:B:202:GLN:O	1:B:206:GLU:HG3	1.76	0.84
1:C:244:THR:HG22	1:C:247:GLN:CG	2.06	0.84
1:L:78:LEU:O	1:L:106:ILE:HD12	1.76	0.84
1:Q:159:SER:HB3	1:R:1:ALA:H3	1.43	0.84
1:A:42:ARG:HD3	1:A:357:PHE:HB3	1.59	0.84
1:N:244:THR:HG22	1:N:247:GLN:N	1.92	0.84
1:F:68:SER:O	1:F:71:GLN:HB2	1.78	0.84
1:G:18:ILE:HD13	1:G:143:ASP:HB3	1.57	0.84
1:L:190:VAL:H	1:L:231:ASN:HD22	1.22	0.84
1:P:223:LEU:O	1:P:226:THR:HB	1.78	0.84
1:A:45:ARG:NH2	1:A:358:THR:H	1.75	0.83
1:E:87:ASP:OD1	1:E:89:GLN:CB	2.26	0.83
1:I:68:SER:CA	1:I:70:ASN:ND2	2.41	0.83
1:K:199:GLU:HB2	3:K:546:HOH:O	1.78	0.83
1:E:351:ALA:O	1:E:352:SER:HB2	1.76	0.83
1:M:123:THR:HG22	1:M:124:ILE:H	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:244:THR:CG2	1:N:247:GLN:H	1.90	0.83
1:M:68:SER:CA	1:M:69:ILE:CD1	2.56	0.83
1:C:224:GLU:N	1:C:224:GLU:OE1	2.11	0.83
1:G:51:THR:CG2	1:G:54:ASN:H	1.92	0.83
1:H:253:VAL:HG12	1:H:291:LEU:HD23	1.58	0.83
1:N:244:THR:HG22	1:N:247:GLN:CG	2.08	0.83
1:M:214:LYS:HE3	1:M:218:ASP:OD1	1.78	0.83
1:O:51:THR:HG22	1:O:54:ASN:H	1.41	0.83
1:Q:50:ASN:HD21	1:Q:55:ARG:HH11	1.23	0.83
1:P:303:ARG:HH21	1:P:357:PHE:CA	1.90	0.83
1:Q:50:ASN:HD21	1:Q:55:ARG:HD3	1.42	0.83
1:A:50:ASN:ND2	1:A:55:ARG:NH1	2.26	0.82
1:D:244:THR:HG22	1:D:247:GLN:N	1.93	0.82
1:G:87:ASP:HB3	1:G:89:GLN:N	1.92	0.82
1:L:281:LEU:HD23	1:L:342:TYR:HE2	1.45	0.82
1:N:313:TRP:CZ2	1:N:315:GLY:HA2	2.14	0.82
1:F:352:SER:OG	1:F:356:LEU:HD21	1.79	0.82
1:J:70:ASN:ND2	1:J:100:LYS:O	2.11	0.82
1:M:68:SER:CB	1:M:69:ILE:HD12	2.07	0.82
1:R:155:ASP:OD1	1:R:156:GLN:HG2	1.79	0.82
1:J:330:ARG:NH1	1:J:346:GLY:HA3	1.95	0.82
1:A:118:THR:HA	1:B:1:ALA:HB3	1.60	0.82
1:E:51:THR:CG2	1:E:54:ASN:H	1.93	0.82
1:I:58:PHE:CZ	1:I:310:LEU:HD13	2.15	0.82
1:J:58:PHE:CZ	1:J:310:LEU:HD13	2.14	0.82
1:J:355:SER:N	3:J:501:HOH:O	2.13	0.82
1:B:277:GLU:OE2	1:B:342:TYR:OH	1.97	0.82
1:E:329:LYS:CD	1:E:347:SER:HB3	2.09	0.82
1:F:51:THR:CG2	1:F:54:ASN:H	1.92	0.82
1:B:118:THR:HG23	1:B:121:GLU:H	1.43	0.82
1:E:95:ASN:O	1:E:99:GLU:HG3	1.80	0.82
1:A:42:ARG:HD2	1:A:357:PHE:CB	2.10	0.82
1:B:67:SER:O	1:B:68:SER:C	2.15	0.82
1:H:330:ARG:NH1	1:H:347:SER:CB	2.43	0.82
1:I:118:THR:CG2	1:I:121:GLU:H	1.92	0.82
1:H:250:MET:HE1	1:H:291:LEU:HD22	1.62	0.81
1:J:329:LYS:HD3	1:J:347:SER:HA	1.60	0.81
1:F:50:ASN:HD21	1:F:55:ARG:NH1	1.76	0.81
1:G:119:ASN:H	1:H:1:ALA:H3	1.24	0.81
1:G:87:ASP:HB2	1:G:91:LYS:H	1.44	0.81
1:D:70:ASN:N	1:D:70:ASN:CB	2.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:344:HIS:HB3	3:M:551:HOH:O	1.80	0.81
1:E:344:HIS:NE2	3:E:501:HOH:O	2.13	0.81
1:K:156:GLN:HB3	1:L:1:ALA:CB	2.10	0.81
1:K:355:SER:CB	1:O:139:LYS:HE2	2.09	0.81
1:I:313:TRP:CE2	1:I:315:GLY:HA2	2.15	0.81
1:I:313:TRP:CZ2	1:I:315:GLY:HA2	2.14	0.81
1:K:355:SER:HB2	1:O:139:LYS:HE2	1.62	0.81
1:D:1:ALA:H2	1:D:220:HIS:CE1	1.98	0.81
1:O:343:VAL:HG23	1:O:344:HIS:N	1.95	0.81
1:Q:51:THR:CG2	1:Q:54:ASN:H	1.92	0.81
1:F:118:THR:HG23	1:F:121:GLU:HB2	1.61	0.81
1:I:2:HIS:O	1:I:3:ARG:O	1.98	0.81
1:L:115:LEU:O	1:L:118:THR:HB	1.81	0.81
1:A:226:THR:CG2	3:A:536:HOH:O	2.28	0.81
1:B:118:THR:CG2	1:B:121:GLU:H	1.93	0.81
1:M:68:SER:HA	1:M:69:ILE:HG13	1.61	0.81
1:N:199:GLU:HB2	3:N:442:HOH:O	1.79	0.81
1:C:189:GLU:HG2	1:C:191:ILE:HD13	1.63	0.81
1:D:274:MET:O	1:D:356:LEU:HD12	1.81	0.80
1:G:58:PHE:CZ	1:G:310:LEU:HD13	2.15	0.80
1:K:66:ASP:OD2	1:K:68:SER:OG	1.97	0.80
1:M:50:ASN:ND2	1:M:55:ARG:HH11	1.79	0.80
1:C:159:SER:HB3	1:D:1:ALA:HB3	1.62	0.80
1:L:58:PHE:CE1	1:L:310:LEU:HD13	2.16	0.80
1:D:191:ILE:CD1	1:D:191:ILE:N	2.44	0.80
1:M:345:THR:HG21	3:M:502:HOH:O	1.82	0.80
1:Q:2:HIS:O	1:Q:3:ARG:CB	2.27	0.80
1:O:70:ASN:HD22	1:O:70:ASN:N	1.77	0.80
1:I:190:VAL:H	1:I:231:ASN:ND2	1.79	0.80
1:O:2:HIS:HB3	1:P:156:GLN:OE1	1.82	0.80
1:B:67:SER:O	1:B:69:ILE:HG22	1.81	0.80
1:C:313:TRP:CZ2	1:C:315:GLY:HA2	2.15	0.80
1:G:244:THR:HG22	1:G:247:GLN:H	1.47	0.80
1:I:1:ALA:HB3	1:J:118:THR:HA	1.62	0.80
1:N:9:GLN:NE2	3:N:401:HOH:O	2.13	0.80
1:P:123:THR:HG22	1:P:124:ILE:H	1.47	0.80
1:N:87:ASP:HB3	1:N:89:GLN:N	1.96	0.80
1:R:87:ASP:OD1	1:R:89:GLN:HB3	1.80	0.80
1:A:307:ALA:HA	1:A:357:PHE:CE2	2.16	0.79
1:E:125:GLN:HE22	1:F:129:GLY:H	1.31	0.79
1:I:2:HIS:HB3	1:J:156:GLN:OE1	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:THR:HG23	3:D:541:HOH:O	1.81	0.79
1:F:118:THR:CG2	1:F:121:GLU:HB2	2.13	0.79
1:F:51:THR:HG22	1:F:54:ASN:H	1.47	0.79
1:I:129:GLY:H	1:J:125:GLN:HE22	1.27	0.79
1:J:71:GLN:CD	3:J:504:HOH:O	2.20	0.79
1:I:119:ASN:N	1:J:1:ALA:HB3	1.95	0.79
1:K:80:HIS:HD2	1:K:137:TYR:OH	1.65	0.79
1:L:8:THR:OG1	1:L:11:GLN:HG3	1.82	0.79
1:M:3:ARG:NH1	1:N:156:GLN:NE2	2.30	0.79
1:M:68:SER:O	1:M:69:ILE:O	1.99	0.79
1:O:123:THR:HG23	1:O:165:GLU:HG3	1.64	0.79
1:D:118:THR:CG2	1:D:121:GLU:H	1.95	0.79
1:H:277:GLU:HG2	1:H:345:THR:HG23	1.63	0.79
1:N:256:LEU:CD1	1:N:267:ILE:HD11	2.11	0.79
1:N:44:GLN:HA	1:N:44:GLN:OE1	1.82	0.79
1:A:2:HIS:HA	1:D:203:TYR:CZ	2.16	0.79
1:K:88:SER:O	1:K:89:GLN:CB	2.26	0.79
1:M:345:THR:CG2	3:M:502:HOH:O	2.31	0.79
1:E:329:LYS:HD3	1:E:347:SER:OG	1.81	0.79
1:N:244:THR:HG23	1:N:246:GLU:H	1.47	0.79
1:D:70:ASN:ND2	1:D:70:ASN:HA	1.67	0.78
1:E:58:PHE:CZ	1:E:310:LEU:HD13	2.18	0.78
1:I:66:ASP:CG	1:I:67:SER:HB2	2.04	0.78
1:B:330:ARG:NE	1:B:330:ARG:HA	1.98	0.78
1:B:89:GLN:O	1:B:91:LYS:N	2.15	0.78
1:C:123:THR:HG21	1:C:165:GLU:OE2	1.83	0.78
1:D:1:ALA:HB2	3:D:531:HOH:O	1.83	0.78
1:J:118:THR:CG2	1:J:121:GLU:H	1.96	0.78
1:B:190:VAL:H	1:B:231:ASN:HD22	1.28	0.78
1:B:250:MET:CE	1:B:291:LEU:HD21	2.13	0.78
1:O:50:ASN:HD21	1:O:55:ARG:HD3	1.49	0.78
1:C:244:THR:HG22	1:C:247:GLN:CB	2.14	0.78
1:M:276:GLU:HG3	1:M:352:SER:HB3	1.64	0.78
1:O:70:ASN:H	1:O:70:ASN:HD22	1.29	0.78
1:R:289:CYS:O	1:R:293:LYS:HE3	1.84	0.78
1:B:203:TYR:HH	1:C:2:HIS:HA	1.46	0.78
1:A:2:HIS:O	1:A:4:PHE:N	2.14	0.77
1:B:342:TYR:CD2	1:B:344:HIS:HA	2.18	0.77
1:P:313:TRP:CE2	1:P:315:GLY:HA2	2.18	0.77
1:Q:3:ARG:HD2	1:R:156:GLN:NE2	2.00	0.77
1:A:342:TYR:CE2	1:A:344:HIS:CB	2.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:ALA:HB3	1:F:159:SER:HB2	1.66	0.77
1:G:129:GLY:H	1:H:125:GLN:HE22	1.30	0.77
1:L:87:ASP:HB2	1:L:91:LYS:N	2.00	0.77
1:E:329:LYS:HZ3	1:E:347:SER:CA	1.96	0.77
1:B:27:LYS:HB3	1:B:72:SER:O	1.83	0.77
1:C:159:SER:HB2	1:D:1:ALA:CB	2.15	0.77
1:G:123:THR:HG23	1:G:165:GLU:HG3	1.65	0.77
1:H:2:HIS:O	1:H:3:ARG:HB2	1.85	0.77
1:M:329:LYS:HZ1	1:M:348:SER:N	1.82	0.77
1:A:203:TYR:HE2	1:D:2:HIS:HD2	1.30	0.77
1:C:303:ARG:HH11	1:C:303:ARG:HG3	1.48	0.77
1:C:65:VAL:O	1:C:100:LYS:NZ	2.17	0.77
1:R:76:VAL:HG23	1:R:102:ILE:HG21	1.66	0.77
1:P:244:THR:CG2	1:P:247:GLN:H	1.97	0.77
1:A:125:GLN:HE21	1:B:128:ASP:HA	1.48	0.77
1:E:276:GLU:HG3	1:E:352:SER:HB3	1.66	0.77
1:N:244:THR:HG23	1:N:246:GLU:N	2.00	0.77
1:H:118:THR:CG2	1:H:121:GLU:H	1.96	0.77
1:O:244:THR:HG22	1:O:247:GLN:N	2.00	0.77
2:A:401:SO4:S	3:A:503:HOH:O	2.42	0.76
1:B:61:ILE:HG21	1:B:323:THR:HG22	1.66	0.76
1:C:159:SER:HB2	1:D:1:ALA:HB3	1.68	0.76
1:H:51:THR:CG2	1:H:54:ASN:H	1.90	0.76
1:J:276:GLU:HG3	1:J:352:SER:HB3	1.67	0.76
1:L:190:VAL:H	1:L:231:ASN:ND2	1.83	0.76
1:O:244:THR:CG2	1:O:247:GLN:H	1.98	0.76
1:Q:156:GLN:HE22	1:R:3:ARG:NE	1.83	0.76
1:A:2:HIS:HB2	1:A:3:ARG:CD	2.14	0.76
1:B:342:TYR:C	1:B:344:HIS:N	2.37	0.76
1:F:226:THR:HG23	3:F:449:HOH:O	1.83	0.76
1:G:244:THR:HG23	1:G:246:GLU:N	2.00	0.76
1:I:271:SER:O	1:I:272:GLY:C	2.20	0.76
1:R:309:ALA:HB1	1:R:323:THR:HG23	1.67	0.76
1:E:329:LYS:CD	1:E:347:SER:CB	2.62	0.76
1:G:123:THR:C	1:G:124:ILE:HD12	2.06	0.76
1:P:80:HIS:HD2	1:P:137:TYR:OH	1.68	0.76
1:Q:200:HIS:HB2	3:Q:2059:HOH:O	1.86	0.76
1:R:330:ARG:HE	1:R:330:ARG:HA	1.50	0.76
1:B:29:ILE:HB	1:B:300:SER:HB2	1.67	0.76
1:E:191:ILE:HB	1:E:192:PRO:HD2	1.68	0.76
1:G:125:GLN:NE2	1:H:129:GLY:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:ASN:ND2	1:K:55:ARG:HH11	1.83	0.76
1:M:343:VAL:CG2	1:M:344:HIS:O	2.27	0.76
1:M:68:SER:O	1:M:68:SER:OG	1.89	0.76
1:H:329:LYS:HD2	1:H:347:SER:CA	2.13	0.76
1:M:2:HIS:O	1:M:4:PHE:HB2	1.85	0.76
1:N:115:LEU:O	1:N:118:THR:HB	1.85	0.76
1:D:273:GLY:HA2	1:D:356:LEU:HB2	1.68	0.75
1:N:123:THR:CG2	1:N:124:ILE:H	1.92	0.75
1:N:2:HIS:HA	1:N:3:ARG:NH1	2.00	0.75
1:P:45:ARG:HH12	1:P:356:LEU:HA	1.51	0.75
1:I:44:GLN:OE1	1:I:44:GLN:HA	1.84	0.75
1:N:58:PHE:CZ	1:N:310:LEU:HD13	2.21	0.75
1:B:67:SER:O	1:B:68:SER:O	2.05	0.75
1:E:89:GLN:NE2	1:E:89:GLN:N	2.30	0.75
1:I:343:VAL:O	1:I:344:HIS:ND1	2.19	0.75
1:L:155:ASP:O	1:L:156:GLN:HB2	1.85	0.75
1:Q:267:ILE:HG12	1:Q:297:LEU:HD23	1.68	0.75
1:A:42:ARG:CD	1:A:357:PHE:CB	2.64	0.75
1:D:51:THR:HG22	1:D:54:ASN:N	2.00	0.75
1:D:58:PHE:CE2	1:D:310:LEU:HD13	2.21	0.75
1:N:1:ALA:O	1:N:3:ARG:NE	2.19	0.75
1:F:267:ILE:HG12	1:F:297:LEU:HD23	1.67	0.75
1:N:65:VAL:HG11	1:N:69:ILE:HG12	1.67	0.75
1:A:154:ALA:HB3	1:A:157:CYS:HB2	1.67	0.75
1:K:156:GLN:HB3	1:L:1:ALA:HB3	1.68	0.75
1:E:88:SER:O	1:E:89:GLN:NE2	2.19	0.75
1:H:124:ILE:HG22	1:H:147:TRP:CZ2	2.21	0.75
1:J:329:LYS:HD3	1:J:347:SER:CA	2.16	0.75
1:O:58:PHE:CE1	1:O:310:LEU:HD13	2.22	0.75
1:Q:4:PHE:HE1	1:R:156:GLN:HG3	1.51	0.75
1:K:51:THR:CG2	1:K:54:ASN:H	1.95	0.74
1:A:118:THR:CG2	1:A:121:GLU:H	2.00	0.74
1:A:226:THR:HG23	3:A:536:HOH:O	1.86	0.74
1:B:58:PHE:CZ	1:B:62:LEU:HD21	2.21	0.74
1:H:80:HIS:HD2	1:H:137:TYR:OH	1.69	0.74
1:M:244:THR:HG23	1:M:247:GLN:HG3	1.68	0.74
1:M:67:SER:O	1:M:69:ILE:N	2.14	0.74
1:Q:1:ALA:O	1:Q:2:HIS:HB2	1.88	0.74
1:B:51:THR:HG22	1:B:54:ASN:N	2.00	0.74
1:P:199:GLU:HB2	3:P:540:HOH:O	1.88	0.74
1:A:125:GLN:NE2	1:B:128:ASP:HA	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:TRP:CE2	1:G:315:GLY:HA2	2.21	0.74
1:H:36:VAL:HG13	1:H:55:ARG:NH1	2.03	0.74
1:K:226:THR:CG2	3:K:512:HOH:O	2.34	0.74
1:L:50:ASN:HD21	1:L:55:ARG:HH11	1.35	0.74
1:P:226:THR:CG2	3:P:520:HOH:O	2.36	0.74
1:C:244:THR:HG23	1:C:247:GLN:H	1.52	0.74
1:O:118:THR:HA	1:P:1:ALA:N	2.03	0.74
1:H:123:THR:C	1:H:124:ILE:HD12	2.07	0.74
1:G:190:VAL:H	1:G:231:ASN:ND2	1.85	0.74
1:I:67:SER:OG	1:I:68:SER:HB2	1.88	0.74
1:A:168:ASN:O	1:A:171:ALA:HB3	1.88	0.73
1:B:342:TYR:CZ	1:B:344:HIS:HA	2.23	0.73
1:E:276:GLU:OE1	1:E:330:ARG:HD3	1.88	0.73
1:G:68:SER:O	1:G:71:GLN:HB2	1.87	0.73
1:G:87:ASP:HB2	1:G:91:LYS:N	2.03	0.73
1:K:65:VAL:O	1:K:100:LYS:NZ	2.17	0.73
1:Q:50:ASN:ND2	1:Q:55:ARG:NH1	2.35	0.73
1:I:118:THR:CA	1:J:1:ALA:H3	2.00	0.73
1:N:344:HIS:H	1:N:344:HIS:CD2	2.01	0.73
1:P:244:THR:HG22	1:P:247:GLN:N	2.02	0.73
1:F:50:ASN:HD21	1:F:55:ARG:HD3	1.53	0.73
1:I:51:THR:HG22	1:I:53:GLU:H	1.54	0.73
1:C:244:THR:HG22	1:C:247:GLN:HB2	1.71	0.73
1:C:50:ASN:ND2	1:C:55:ARG:HH11	1.85	0.73
1:I:118:THR:CA	1:J:1:ALA:H2	1.97	0.73
1:L:12:LYS:HE2	1:L:222:TYR:CD1	2.23	0.73
1:O:3:ARG:HG2	1:O:4:PHE:N	2.03	0.73
1:D:2:HIS:O	1:D:3:ARG:HB3	1.87	0.73
1:P:42:ARG:HH12	1:P:358:THR:CB	2.01	0.73
1:H:89:GLN:O	1:H:91:LYS:N	2.20	0.73
1:O:67:SER:O	1:O:70:ASN:ND2	2.22	0.73
1:A:355:SER:O	1:A:356:LEU:HD23	1.89	0.73
3:J:564:HOH:O	1:K:200:HIS:HB2	1.89	0.73
1:M:2:HIS:O	1:M:3:ARG:C	2.27	0.73
1:O:156:GLN:O	1:P:1:ALA:HB1	1.89	0.73
1:Q:58:PHE:CZ	1:Q:310:LEU:HD13	2.24	0.73
1:E:244:THR:HG22	1:E:247:GLN:N	2.04	0.72
1:Q:55:ARG:O	1:Q:59:ARG:HG2	1.89	0.72
1:E:250:MET:CE	1:E:291:LEU:CD2	2.66	0.72
1:F:244:THR:CG2	1:F:247:GLN:H	2.02	0.72
1:L:89:GLN:O	1:L:89:GLN:CG	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:ARG:NH1	1:J:347:SER:H	1.86	0.72
1:C:129:GLY:H	1:D:125:GLN:HE22	1.36	0.72
1:G:3:ARG:HG2	1:G:3:ARG:HH11	1.53	0.72
1:D:244:THR:HG23	1:D:246:GLU:H	1.54	0.72
1:E:256:LEU:HD13	1:E:267:ILE:CD1	2.15	0.72
1:E:58:PHE:CE1	1:E:310:LEU:HD13	2.25	0.72
1:D:86:LYS:HD3	1:D:90:GLY:HA3	1.71	0.72
1:O:220:HIS:HE1	3:O:528:HOH:O	1.72	0.72
1:P:352:SER:N	3:P:501:HOH:O	2.22	0.72
1:H:50:ASN:HD21	1:H:55:ARG:HD3	1.53	0.72
1:I:115:LEU:O	1:I:118:THR:HB	1.90	0.72
1:H:62:LEU:O	1:H:65:VAL:HG13	1.89	0.72
1:H:250:MET:HE1	1:H:291:LEU:CD2	2.20	0.72
1:K:88:SER:O	1:K:89:GLN:HB2	1.88	0.72
1:N:50:ASN:ND2	1:N:55:ARG:HH11	1.87	0.72
1:B:244:THR:HG22	1:B:247:GLN:N	2.04	0.72
1:C:129:GLY:H	1:D:125:GLN:NE2	1.88	0.72
1:C:156:GLN:NE2	1:D:3:ARG:HD2	2.04	0.72
1:I:322:ALA:O	1:I:325:GLU:HB2	1.90	0.71
1:J:330:ARG:CZ	1:J:346:GLY:HA3	2.20	0.71
1:N:78:LEU:O	1:N:106:ILE:HD12	1.90	0.71
1:C:244:THR:CG2	1:C:247:GLN:HG3	2.20	0.71
1:E:256:LEU:CD1	1:E:267:ILE:HD11	2.15	0.71
1:F:190:VAL:H	1:F:231:ASN:ND2	1.87	0.71
1:G:244:THR:HB	1:G:247:GLN:HE21	1.54	0.71
1:H:256:LEU:CD1	1:H:267:ILE:HD11	2.15	0.71
1:I:34:GLU:HB2	1:I:38:THR:HB	1.72	0.71
1:J:230:PRO:HG3	1:J:267:ILE:CD1	2.20	0.71
1:P:42:ARG:HH12	1:P:358:THR:HB	1.53	0.71
1:E:303:ARG:CG	1:E:303:ARG:HH11	2.03	0.71
1:G:313:TRP:CZ2	1:G:315:GLY:HA2	2.24	0.71
1:G:70:ASN:ND2	1:G:100:LYS:O	2.22	0.71
1:O:59:ARG:HB3	1:O:63:PHE:CE1	2.24	0.71
1:B:244:THR:HG22	1:B:247:GLN:HG3	1.73	0.71
1:E:2:HIS:HB3	1:F:156:GLN:CD	2.09	0.71
1:H:172:ARG:NH2	1:H:176:ILE:HD11	2.04	0.71
1:I:119:ASN:H	1:J:1:ALA:CB	1.97	0.71
1:A:9:GLN:NE2	3:A:504:HOH:O	2.22	0.71
1:B:250:MET:HE3	1:B:291:LEU:CD2	2.15	0.71
1:A:303:ARG:CG	1:A:357:PHE:HD1	2.04	0.71
1:A:203:TYR:HE2	1:D:2:HIS:CD2	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ALA:HB3	1:D:118:THR:HA	1.72	0.71
1:F:274:MET:O	1:F:356:LEU:HD12	1.90	0.71
1:N:224:GLU:OE1	1:N:224:GLU:N	2.20	0.71
1:R:226:THR:CG2	3:R:520:HOH:O	2.39	0.71
1:A:191:ILE:HB	1:A:192:PRO:HD2	1.73	0.71
1:A:118:THR:HA	1:B:1:ALA:HB2	1.72	0.71
1:E:129:GLY:H	1:F:125:GLN:HE22	1.37	0.71
1:G:51:THR:HG22	1:G:54:ASN:H	1.54	0.71
1:I:123:THR:HG22	1:I:124:ILE:N	2.04	0.71
1:L:50:ASN:ND2	1:L:55:ARG:HH11	1.87	0.71
1:N:2:HIS:HA	1:N:3:ARG:NH2	2.05	0.71
1:O:58:PHE:CZ	1:O:310:LEU:HD13	2.25	0.71
1:P:276:GLU:HB2	1:P:352:SER:HB3	1.73	0.71
1:J:330:ARG:HH11	1:J:347:SER:H	1.38	0.71
1:L:220:HIS:HE1	3:L:407:HOH:O	1.72	0.71
1:M:345:THR:OG1	3:M:502:HOH:O	2.08	0.71
1:O:115:LEU:O	1:O:118:THR:HB	1.91	0.70
1:Q:156:GLN:NE2	1:R:3:ARG:NE	2.39	0.70
1:B:244:THR:HG21	3:B:414:HOH:O	1.90	0.70
1:B:254:THR:O	1:B:258:ARG:HG2	1.91	0.70
1:C:271:SER:HB3	1:C:301:TYR:CE2	2.26	0.70
1:D:223:LEU:O	1:D:226:THR:HB	1.90	0.70
1:D:89:GLN:O	1:D:91:LYS:N	2.23	0.70
1:A:42:ARG:HD3	1:A:357:PHE:O	1.90	0.70
1:E:253:VAL:CG1	1:E:291:LEU:HD23	2.20	0.70
1:E:89:GLN:HB2	1:E:89:GLN:OE1	1.89	0.70
1:L:2:HIS:O	1:L:3:ARG:O	2.08	0.70
1:M:345:THR:CG2	1:M:347:SER:HB3	2.21	0.70
1:F:223:LEU:O	1:F:226:THR:HB	1.90	0.70
1:M:50:ASN:HD21	1:M:55:ARG:HH11	1.39	0.70
1:N:284:ASN:HD22	1:N:340:GLY:HA2	1.56	0.70
1:J:329:LYS:NZ	1:J:347:SER:HA	2.06	0.70
1:K:345:THR:O	1:K:346:GLY:O	2.08	0.70
1:B:51:THR:O	1:B:55:ARG:HG3	1.92	0.70
1:E:50:ASN:HD21	1:E:55:ARG:HD3	1.56	0.70
1:L:58:PHE:CZ	1:L:62:LEU:HD21	2.27	0.70
1:L:87:ASP:CB	1:L:91:LYS:H	2.01	0.70
1:O:254:THR:O	1:O:258:ARG:HG2	1.92	0.70
1:P:12:LYS:HB3	1:P:222:TYR:CZ	2.26	0.70
1:B:61:ILE:HG21	1:B:323:THR:HG21	1.72	0.70
1:E:4:PHE:O	1:F:117:GLY:HA2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:202:GLN:HB2	1:N:233:VAL:HG11	1.73	0.70
1:E:329:LYS:NZ	1:E:347:SER:CA	2.54	0.70
1:I:50:ASN:ND2	1:I:55:ARG:HH11	1.90	0.70
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.74	0.70
1:N:244:THR:CG2	1:N:247:GLN:N	2.53	0.70
1:O:319:ASN:O	1:O:320:LYS:C	2.26	0.70
1:B:190:VAL:H	1:B:231:ASN:ND2	1.89	0.70
1:C:244:THR:HG22	1:C:247:GLN:HG3	1.73	0.70
1:C:254:THR:O	1:C:258:ARG:HG2	1.92	0.70
1:H:226:THR:CG2	3:H:421:HOH:O	2.40	0.70
1:Q:190:VAL:H	1:Q:231:ASN:ND2	1.90	0.70
1:Q:250:MET:O	1:Q:250:MET:HG3	1.90	0.70
1:C:237:HIS:CG	3:C:403:HOH:O	2.45	0.69
1:E:78:LEU:O	1:E:106:ILE:HD12	1.92	0.69
1:H:329:LYS:CE	1:H:347:SER:HA	2.21	0.69
1:I:50:ASN:HD21	1:I:55:ARG:HD3	1.58	0.69
1:P:250:MET:CE	1:P:291:LEU:HD11	2.21	0.69
1:E:240:THR:O	1:E:242:LYS:HE3	1.92	0.69
1:F:351:ALA:O	1:F:352:SER:CB	2.40	0.69
1:H:354:GLN:HG2	1:H:356:LEU:CD2	2.22	0.69
1:J:95:ASN:O	1:J:99:GLU:HG3	1.91	0.69
1:P:250:MET:HE3	1:P:291:LEU:HD11	1.75	0.69
1:Q:256:LEU:HD13	1:Q:267:ILE:HD11	1.73	0.69
1:Q:4:PHE:CE1	1:R:156:GLN:HG3	2.27	0.69
1:B:80:HIS:HD2	1:B:137:TYR:OH	1.75	0.69
1:C:2:HIS:HB2	1:D:156:GLN:OE1	1.92	0.69
1:I:320:LYS:O	1:I:324:GLN:HG3	1.93	0.69
1:M:67:SER:C	1:M:69:ILE:H	1.82	0.69
1:O:129:GLY:H	1:P:125:GLN:HE22	1.39	0.69
1:P:50:ASN:ND2	1:P:55:ARG:HH11	1.90	0.69
1:B:61:ILE:HG23	1:B:324:GLN:HG2	1.74	0.69
1:N:202:GLN:O	1:N:206:GLU:HG3	1.93	0.69
1:R:214:LYS:HD2	1:R:214:LYS:O	1.91	0.69
1:A:207:LYS:HE2	1:D:2:HIS:HE2	1.55	0.69
1:D:87:ASP:HB2	1:D:91:LYS:N	2.07	0.69
1:E:344:HIS:CD2	3:E:501:HOH:O	2.43	0.69
1:M:159:SER:HB3	1:N:1:ALA:HA	1.74	0.69
1:D:351:ALA:O	1:D:354:GLN:HB2	1.91	0.69
1:E:87:ASP:OD1	1:E:89:GLN:HB2	1.93	0.69
1:D:3:ARG:HD3	3:D:575:HOH:O	1.91	0.69
1:E:344:HIS:CE1	3:E:501:HOH:O	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:THR:HG22	1:E:54:ASN:HB2	1.72	0.69
1:F:51:THR:HG22	1:F:54:ASN:HB2	1.74	0.69
1:H:172:ARG:O	1:H:176:ILE:HG13	1.93	0.69
1:R:115:LEU:O	1:R:118:THR:HB	1.93	0.69
1:C:87:ASP:HB3	1:C:89:GLN:N	2.08	0.69
1:G:118:THR:CG2	1:G:121:GLU:H	2.06	0.69
1:L:244:THR:HG22	1:L:247:GLN:CB	2.22	0.69
1:N:1:ALA:O	1:N:3:ARG:CZ	2.40	0.69
1:C:51:THR:HG23	1:C:53:GLU:H	1.57	0.69
1:M:58:PHE:CZ	1:M:310:LEU:HD13	2.27	0.69
1:O:50:ASN:ND2	1:O:55:ARG:HH11	1.91	0.69
1:E:28:GLY:HA3	1:E:299:PHE:CZ	2.28	0.69
1:G:244:THR:HG23	1:G:246:GLU:H	1.56	0.69
1:H:223:LEU:O	1:H:226:THR:HB	1.93	0.69
1:I:67:SER:CB	3:I:406:HOH:O	2.41	0.69
1:K:244:THR:CG2	1:K:247:GLN:N	2.40	0.69
1:M:115:LEU:O	1:M:118:THR:HB	1.93	0.69
1:O:1:ALA:HA	3:O:528:HOH:O	1.92	0.69
1:R:244:THR:HG22	1:R:247:GLN:N	1.98	0.69
1:A:277:GLU:CD	1:A:347:SER:HB2	2.13	0.69
1:G:118:THR:HG23	1:G:121:GLU:H	1.58	0.69
1:K:355:SER:HB2	1:O:139:LYS:CE	2.23	0.69
1:I:65:VAL:CG1	1:I:69:ILE:HD13	2.21	0.68
1:N:200:HIS:CE1	1:O:2:HIS:NE2	2.61	0.68
1:A:271:SER:OG	3:A:503:HOH:O	2.03	0.68
1:I:12:LYS:HG2	1:I:222:TYR:CZ	2.27	0.68
1:P:290:PRO:O	1:P:291:LEU:HG	1.92	0.68
1:J:276:GLU:CG	1:J:352:SER:HB3	2.23	0.68
1:L:87:ASP:HB3	1:L:89:GLN:N	2.05	0.68
1:M:119:ASN:H	1:N:1:ALA:HB3	1.57	0.68
1:M:350:ALA:H	1:M:353:THR:CG2	2.06	0.68
1:D:50:ASN:ND2	1:D:55:ARG:HH11	1.90	0.68
1:I:244:THR:HG23	1:I:246:GLU:H	1.59	0.68
1:L:118:THR:HG23	1:L:121:GLU:H	1.58	0.68
1:M:228:LEU:HG	1:M:230:PRO:HD3	1.74	0.68
1:O:128:ASP:HA	1:P:125:GLN:HE21	1.58	0.68
1:B:187:GLU:HG3	1:B:229:LYS:O	1.92	0.68
1:D:1:ALA:H1	1:D:220:HIS:CE1	2.11	0.68
1:N:274:MET:HE3	1:N:279:ALA:HA	1.75	0.68
1:O:276:GLU:OE2	1:O:307:ALA:HB3	1.93	0.68
1:B:2:HIS:NE2	1:C:200:HIS:CE1	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:HIS:O	1:D:4:PHE:HD1	1.77	0.68
1:F:354:GLN:O	1:F:355:SER:HB2	1.92	0.68
1:I:198:LEU:HD22	1:I:243:TYR:CD2	2.29	0.68
1:A:124:ILE:CD1	1:A:149:ALA:HA	2.22	0.68
1:B:244:THR:CG2	1:B:247:GLN:HG3	2.23	0.68
1:B:313:TRP:CZ2	1:B:315:GLY:HA2	2.28	0.68
1:C:36:VAL:O	1:C:36:VAL:HG12	1.93	0.68
1:L:51:THR:HG22	1:L:54:ASN:HB2	1.76	0.68
1:N:189:GLU:HG2	1:N:191:ILE:HD12	1.75	0.68
1:I:36:VAL:HG12	1:I:36:VAL:O	1.91	0.68
1:I:51:THR:HG22	1:I:54:ASN:H	1.57	0.68
1:I:67:SER:OG	1:I:68:SER:CB	2.42	0.68
1:N:190:VAL:H	1:N:231:ASN:HD22	1.40	0.68
1:R:124:ILE:HG21	1:R:147:TRP:NE1	2.09	0.68
1:R:257:HIS:CD2	1:R:292:PRO:HD2	2.28	0.68
1:A:303:ARG:HG2	1:A:357:PHE:HB2	1.74	0.68
1:C:191:ILE:HD13	1:C:191:ILE:N	2.07	0.68
1:M:189:GLU:CG	1:M:191:ILE:HD13	2.23	0.68
1:R:223:LEU:O	1:R:226:THR:HB	1.94	0.68
1:B:313:TRP:CE2	1:B:315:GLY:HA2	2.29	0.68
1:D:329:LYS:HZ3	1:D:347:SER:HA	1.56	0.68
1:K:128:ASP:HB2	1:L:128:ASP:OD2	1.93	0.68
1:N:118:THR:CG2	1:N:121:GLU:H	2.07	0.68
1:O:18:ILE:HD13	1:O:143:ASP:HB3	1.76	0.68
1:O:330:ARG:HE	1:O:330:ARG:HA	1.59	0.68
1:O:343:VAL:O	1:O:344:HIS:ND1	2.27	0.68
1:B:344:HIS:CG	1:B:345:THR:N	2.61	0.67
1:B:2:HIS:NE2	1:C:200:HIS:HE1	1.91	0.67
1:F:214:LYS:HE3	1:F:218:ASP:OD1	1.94	0.67
1:F:354:GLN:O	1:F:355:SER:CB	2.42	0.67
1:I:150:VAL:HG13	1:I:191:ILE:HG13	1.76	0.67
1:I:53:GLU:OE1	1:I:53:GLU:HA	1.94	0.67
1:M:353:THR:HG23	1:M:353:THR:O	1.94	0.67
1:D:87:ASP:CB	1:D:91:LYS:H	2.04	0.67
1:J:170:LEU:HD22	1:J:186:VAL:HG13	1.76	0.67
1:K:44:GLN:OE1	1:K:44:GLN:HA	1.93	0.67
1:I:51:THR:CG2	1:I:53:GLU:H	2.07	0.67
1:L:244:THR:HG22	1:L:247:GLN:HB2	1.76	0.67
1:D:87:ASP:HB3	1:D:89:GLN:O	1.93	0.67
1:E:271:SER:HA	1:E:274:MET:CE	2.23	0.67
1:R:244:THR:CG2	1:R:247:GLN:H	2.00	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:SER:CA	1:I:70:ASN:HD22	2.04	0.67
1:L:2:HIS:O	1:L:3:ARG:C	2.33	0.67
1:N:118:THR:CG2	1:N:121:GLU:HB2	2.24	0.67
1:C:190:VAL:H	1:C:231:ASN:ND2	1.92	0.67
1:E:190:VAL:H	1:E:231:ASN:HD22	1.39	0.67
1:O:190:VAL:H	1:O:231:ASN:ND2	1.91	0.67
1:E:51:THR:HG22	1:E:54:ASN:CB	2.23	0.67
1:G:58:PHE:CE1	1:G:310:LEU:HD13	2.29	0.67
1:H:257:HIS:HD2	1:H:292:PRO:HD2	1.59	0.67
1:H:87:ASP:OD2	1:H:89:GLN:O	2.13	0.67
1:I:202:GLN:O	1:I:206:GLU:HG3	1.95	0.67
1:K:58:PHE:CZ	1:K:310:LEU:HD13	2.29	0.67
1:M:69:ILE:CD1	1:M:328:MET:HE1	2.20	0.67
1:M:329:LYS:HE3	1:M:347:SER:CB	2.12	0.67
1:N:80:HIS:HD2	1:N:137:TYR:OH	1.76	0.67
1:F:50:ASN:ND2	1:F:55:ARG:NH1	2.35	0.67
1:N:68:SER:O	1:N:70:ASN:N	2.27	0.67
1:A:123:THR:HG23	1:A:165:GLU:HG3	1.77	0.67
1:D:244:THR:HB	1:D:247:GLN:OE1	1.95	0.67
1:M:128:ASP:HB2	1:N:128:ASP:OD2	1.93	0.67
1:Q:271:SER:HA	1:Q:274:MET:HE3	1.76	0.67
1:G:33:ASP:HB3	1:G:77:ILE:HG22	1.77	0.67
1:P:303:ARG:NH2	1:P:357:PHE:CD1	2.53	0.67
1:E:303:ARG:HH11	1:E:303:ARG:HG3	1.60	0.66
1:M:118:THR:HA	1:N:1:ALA:HB3	1.76	0.66
1:N:94:ARG:O	1:N:98:LYS:HG3	1.94	0.66
1:A:67:SER:CA	3:A:502:HOH:O	2.33	0.66
1:B:274:MET:HE3	1:B:279:ALA:HB2	1.77	0.66
1:B:60:GLU:OE1	1:B:87:ASP:HB2	1.95	0.66
1:M:189:GLU:HG2	1:M:191:ILE:HD13	1.77	0.66
1:P:28:GLY:HA3	1:P:299:PHE:CZ	2.30	0.66
1:Q:256:LEU:HD13	1:Q:267:ILE:CD1	2.26	0.66
1:I:277:GLU:O	1:I:281:LEU:HG	1.95	0.66
1:A:118:THR:HG23	1:A:121:GLU:H	1.60	0.66
1:B:207:LYS:CE	1:C:2:HIS:HE2	2.07	0.66
1:C:50:ASN:HD21	1:C:55:ARG:HD3	1.59	0.66
1:I:170:LEU:HD22	1:I:186:VAL:HG13	1.75	0.66
1:L:118:THR:CG2	1:L:121:GLU:N	2.53	0.66
1:L:281:LEU:HD23	1:L:342:TYR:CE2	2.29	0.66
1:M:16:SER:O	1:M:20:GLN:HG3	1.93	0.66
1:N:189:GLU:HG2	1:N:191:ILE:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:226:THR:CG2	3:Q:2024:HOH:O	2.43	0.66
1:D:148:ARG:HA	1:D:187:GLU:HB3	1.78	0.66
1:E:202:GLN:HB2	1:E:233:VAL:HG11	1.78	0.66
1:E:250:MET:HE1	1:E:291:LEU:CD2	2.21	0.66
1:M:68:SER:C	1:M:69:ILE:CG1	2.42	0.66
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.77	0.66
1:C:159:SER:CB	1:D:1:ALA:CB	2.73	0.66
1:H:195:ASP:O	1:H:239:CYS:HB2	1.96	0.66
1:M:329:LYS:HZ1	1:M:347:SER:C	1.98	0.66
1:G:125:GLN:HE22	1:H:129:GLY:H	1.42	0.66
1:H:257:HIS:CD2	1:H:292:PRO:HD2	2.30	0.66
1:R:124:ILE:CG2	1:R:147:TRP:CZ2	2.77	0.66
1:B:272:GLY:HA2	1:B:303:ARG:NH1	2.10	0.66
1:C:87:ASP:CB	1:C:89:GLN:H	2.05	0.66
1:K:88:SER:O	1:K:89:GLN:CG	2.44	0.66
1:M:1:ALA:N	1:N:118:THR:CB	2.59	0.66
1:M:1:ALA:H3	1:N:119:ASN:N	1.94	0.66
1:N:200:HIS:HE1	1:O:2:HIS:NE2	1.94	0.66
1:Q:118:THR:HG21	1:Q:121:GLU:HB2	1.77	0.66
1:R:240:THR:O	1:R:242:LYS:HE3	1.95	0.66
1:R:80:HIS:HD2	1:R:137:TYR:OH	1.78	0.66
1:B:244:THR:CG2	1:B:247:GLN:N	2.59	0.66
1:E:89:GLN:OE1	1:E:89:GLN:HB3	1.89	0.66
1:K:8:THR:N	1:K:11:GLN:OE1	2.24	0.66
1:M:119:ASN:HB2	1:N:4:PHE:CE1	2.31	0.66
1:Q:218:ASP:O	1:R:161:LEU:HD22	1.96	0.66
1:Q:121:GLU:OE1	1:R:1:ALA:HB3	1.95	0.66
1:A:128:ASP:OD2	1:B:128:ASP:HB2	1.96	0.66
1:B:50:ASN:ND2	1:B:55:ARG:HD3	2.07	0.66
1:D:123:THR:HG23	1:D:165:GLU:HG3	1.78	0.66
1:G:118:THR:HG21	1:G:121:GLU:HB2	1.78	0.66
1:I:330:ARG:HE	1:I:330:ARG:HA	1.60	0.66
1:B:207:LYS:CE	1:C:2:HIS:NE2	2.60	0.65
1:D:329:LYS:HD3	1:D:347:SER:CB	2.27	0.65
1:I:159:SER:O	1:I:163:ILE:HG13	1.96	0.65
1:L:48:VAL:CG1	1:L:54:ASN:ND2	2.59	0.65
1:N:8:THR:OG1	1:N:11:GLN:HG3	1.95	0.65
1:P:237:HIS:HE1	3:P:541:HOH:O	1.79	0.65
1:E:38:THR:O	1:E:42:ARG:HG2	1.96	0.65
1:K:125:GLN:HE22	1:L:129:GLY:H	1.43	0.65
1:L:202:GLN:O	1:L:206:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:271:SER:HA	1:O:274:MET:CE	2.26	0.65
1:R:67:SER:O	1:R:70:ASN:HB2	1.96	0.65
1:A:187:GLU:HB2	1:A:229:LYS:HB3	1.78	0.65
1:B:342:TYR:CD2	1:B:344:HIS:CA	2.80	0.65
1:B:50:ASN:ND2	1:B:55:ARG:HH11	1.93	0.65
1:G:240:THR:O	1:G:242:LYS:HE3	1.95	0.65
1:I:12:LYS:HG2	1:I:222:TYR:CE1	2.31	0.65
1:E:343:VAL:O	1:E:344:HIS:HB2	1.96	0.65
1:H:244:THR:N	1:H:247:GLN:OE1	2.29	0.65
1:F:256:LEU:HD11	1:F:267:ILE:HD11	1.78	0.65
1:F:277:GLU:OE2	1:F:344:HIS:ND1	2.27	0.65
1:G:244:THR:CG2	1:G:247:GLN:H	2.09	0.65
1:J:223:LEU:O	1:J:226:THR:HB	1.95	0.65
1:L:123:THR:HG23	1:L:165:GLU:HG3	1.78	0.65
1:N:203:TYR:CZ	1:O:2:HIS:HA	2.32	0.65
1:C:36:VAL:HG13	1:C:55:ARG:NH1	2.12	0.65
1:H:112:GLY:HA2	1:H:123:THR:O	1.97	0.65
1:I:156:GLN:HB3	1:J:1:ALA:HB1	1.77	0.65
1:O:202:GLN:O	1:O:206:GLU:HG3	1.96	0.65
1:A:220:HIS:HE1	3:A:559:HOH:O	1.80	0.65
1:A:3:ARG:HD3	1:B:156:GLN:OE1	1.96	0.65
1:C:244:THR:CG2	1:C:247:GLN:H	2.08	0.65
1:G:3:ARG:NE	1:H:156:GLN:NE2	2.44	0.65
1:K:223:LEU:O	1:K:226:THR:HB	1.96	0.65
1:L:184:PRO:HD2	1:L:225:GLY:O	1.97	0.65
1:K:353:THR:HG21	1:O:92:LEU:HD11	1.79	0.65
1:R:124:ILE:HG21	1:R:147:TRP:CE2	2.31	0.65
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.32	0.65
1:C:125:GLN:NE2	1:D:129:GLY:H	1.95	0.65
1:F:244:THR:HG22	1:F:247:GLN:HB2	1.77	0.65
1:A:58:PHE:CZ	1:A:310:LEU:HD13	2.32	0.65
1:E:89:GLN:N	1:E:89:GLN:HE22	1.95	0.65
1:G:188:PRO:O	1:G:188:PRO:HG2	1.97	0.65
1:I:244:THR:HG23	1:I:246:GLU:N	2.11	0.65
1:N:192:PRO:HD3	3:N:428:HOH:O	1.97	0.65
1:Q:87:ASP:OD2	1:Q:88:SER:N	2.30	0.65
1:R:244:THR:HG22	1:R:247:GLN:HG3	1.79	0.65
1:A:244:THR:HB	1:A:247:GLN:OE1	1.97	0.65
1:C:231:ASN:H	1:C:231:ASN:ND2	1.95	0.65
1:N:313:TRP:CD2	1:N:315:GLY:HA2	2.32	0.65
1:A:156:GLN:HE22	1:B:3:ARG:NE	1.93	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:GLN:H	1:E:89:GLN:NE2	1.93	0.64
1:F:256:LEU:CD1	1:F:267:ILE:HD11	2.28	0.64
1:L:254:THR:O	1:L:258:ARG:HG2	1.96	0.64
1:N:118:THR:HG23	1:N:121:GLU:H	1.62	0.64
1:R:36:VAL:HG13	1:R:55:ARG:NH1	2.11	0.64
1:C:118:THR:CG2	1:C:121:GLU:N	2.59	0.64
1:E:191:ILE:HB	1:E:192:PRO:CD	2.26	0.64
1:M:146:LYS:HE2	1:M:187:GLU:OE1	1.97	0.64
1:N:284:ASN:ND2	1:N:340:GLY:HA2	2.11	0.64
1:N:3:ARG:CZ	1:O:203:TYR:CZ	2.80	0.64
1:N:3:ARG:NE	1:O:203:TYR:OH	2.28	0.64
1:O:118:THR:CG2	1:O:121:GLU:HB2	2.26	0.64
1:O:51:THR:HG22	1:O:54:ASN:N	2.12	0.64
1:R:244:THR:CG2	1:R:246:GLU:HB2	2.27	0.64
1:A:191:ILE:HB	1:A:192:PRO:CD	2.28	0.64
1:B:244:THR:HG22	1:B:247:GLN:CG	2.27	0.64
1:H:330:ARG:HH11	1:H:347:SER:HB3	1.62	0.64
1:D:115:LEU:O	1:D:118:THR:HB	1.97	0.64
1:E:115:LEU:O	1:E:118:THR:HB	1.98	0.64
1:H:8:THR:HB	1:H:11:GLN:H	1.62	0.64
1:I:224:GLU:N	1:I:224:GLU:OE1	2.26	0.64
1:I:82:THR:O	1:I:82:THR:HG22	1.97	0.64
1:N:3:ARG:N	1:N:3:ARG:NH1	2.46	0.64
1:Q:320:LYS:O	1:Q:324:GLN:HG3	1.98	0.64
1:A:3:ARG:H	1:A:3:ARG:HD2	1.62	0.64
1:D:198:LEU:CD1	1:D:234:THR:HA	2.28	0.64
1:H:119:ASN:O	1:H:152:ARG:NH1	2.30	0.64
1:O:190:VAL:H	1:O:231:ASN:HD22	1.45	0.64
1:E:124:ILE:HG22	1:E:147:TRP:CZ2	2.33	0.64
1:E:2:HIS:CB	1:F:156:GLN:OE1	2.45	0.64
1:I:197:ASP:C	1:I:197:ASP:OD1	2.34	0.64
1:I:65:VAL:O	1:I:66:ASP:C	2.32	0.64
1:N:118:THR:HG21	1:N:121:GLU:HB2	1.78	0.64
1:N:51:THR:O	1:N:54:ASN:N	2.31	0.64
1:A:45:ARG:HH21	1:A:358:THR:N	1.91	0.64
1:E:50:ASN:ND2	1:E:55:ARG:HH11	1.96	0.64
1:F:80:HIS:HD2	1:F:137:TYR:OH	1.79	0.64
1:Q:313:TRP:CE2	1:Q:315:GLY:HA2	2.32	0.64
1:D:52:GLU:O	1:D:55:ARG:HB2	1.98	0.64
1:M:123:THR:O	1:M:124:ILE:HD13	1.97	0.64
1:M:2:HIS:ND1	1:P:203:TYR:OH	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG23	1:B:324:GLN:HB3	1.80	0.64
1:O:25:ASN:H	1:O:27:LYS:HD2	1.63	0.64
1:Q:156:GLN:HE22	1:R:3:ARG:CD	2.11	0.64
1:Q:244:THR:CG2	1:Q:247:GLN:H	2.10	0.64
1:D:75:GLY:HA2	1:D:103:VAL:O	1.97	0.64
1:N:171:ALA:HA	1:N:216:LEU:HD12	1.79	0.64
1:N:34:GLU:HB3	1:N:38:THR:HB	1.80	0.64
1:Q:313:TRP:CZ2	1:Q:315:GLY:HA2	2.32	0.64
1:A:303:ARG:HB3	1:A:357:PHE:CD1	2.33	0.63
1:H:349:GLY:O	1:H:351:ALA:N	2.31	0.63
1:N:53:GLU:OE1	1:N:53:GLU:HA	1.98	0.63
1:A:203:TYR:CE2	1:D:2:HIS:CD2	2.86	0.63
1:A:202:GLN:O	1:A:206:GLU:HG3	1.98	0.63
1:H:308:SER:HB3	1:H:351:ALA:HB1	1.80	0.63
1:J:276:GLU:HG3	1:J:352:SER:CB	2.27	0.63
1:M:1:ALA:H3	1:N:118:THR:HA	1.51	0.63
1:O:70:ASN:ND2	1:O:70:ASN:H	1.96	0.63
1:F:115:LEU:O	1:F:118:THR:HB	1.98	0.63
1:L:123:THR:HG22	1:L:124:ILE:H	1.63	0.63
1:C:44:GLN:HA	1:C:44:GLN:OE1	1.98	0.63
1:E:329:LYS:CE	1:E:347:SER:CB	2.74	0.63
1:L:244:THR:HG22	1:L:247:GLN:H	1.63	0.63
1:L:319:ASN:O	1:L:320:LYS:C	2.37	0.63
1:P:313:TRP:CZ2	1:P:315:GLY:HA2	2.33	0.63
1:Q:156:GLN:HB3	1:R:1:ALA:N	2.13	0.63
1:A:156:GLN:HE22	1:B:3:ARG:HE	1.47	0.63
1:C:118:THR:HG23	1:C:121:GLU:H	1.59	0.63
1:G:86:LYS:HD3	1:G:90:GLY:HA2	1.81	0.63
1:H:86:LYS:HB3	1:H:90:GLY:HA2	1.79	0.63
1:K:129:GLY:H	1:L:125:GLN:HE22	1.45	0.63
1:L:58:PHE:CZ	1:L:310:LEU:HD13	2.32	0.63
1:M:69:ILE:CD1	1:M:328:MET:CE	2.62	0.63
1:O:244:THR:HG23	1:O:246:GLU:H	1.64	0.63
1:O:342:TYR:CD2	1:O:342:TYR:O	2.51	0.63
1:D:50:ASN:HD21	1:D:55:ARG:HH11	1.46	0.63
1:D:71:GLN:OE1	3:D:501:HOH:O	2.15	0.63
1:G:189:GLU:HG2	1:G:191:ILE:HD12	1.80	0.63
1:I:65:VAL:HG23	1:I:324:GLN:HB3	1.80	0.63
1:Q:109:ASP:HB2	1:Q:124:ILE:HG21	1.80	0.63
1:A:80:HIS:HD2	1:A:137:TYR:OH	1.82	0.63
1:A:349:GLY:O	1:A:352:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:308:SER:CB	1:H:351:ALA:HB1	2.29	0.63
1:J:146:LYS:HE2	1:J:187:GLU:OE1	1.98	0.63
1:M:68:SER:HA	1:M:69:ILE:CD1	2.29	0.63
1:A:343:VAL:C	1:A:344:HIS:O	2.34	0.63
1:A:65:VAL:O	1:A:100:LYS:NZ	2.28	0.63
1:D:123:THR:HG21	1:D:165:GLU:OE2	1.97	0.63
1:P:30:LEU:HB3	1:P:76:VAL:HG22	1.81	0.63
1:A:213:TYR:OH	1:A:228:LEU:HD13	1.99	0.63
1:C:223:LEU:O	1:C:226:THR:HB	1.98	0.63
1:E:87:ASP:O	1:E:89:GLN:CB	2.47	0.63
1:K:123:THR:HG22	1:K:124:ILE:H	1.64	0.63
1:M:121:GLU:OE1	1:N:1:ALA:HB2	1.99	0.63
1:Q:156:GLN:HB3	1:R:1:ALA:CA	2.28	0.63
1:A:303:ARG:CG	1:A:357:PHE:CD1	2.78	0.62
1:I:51:THR:CG2	1:I:54:ASN:H	2.12	0.62
1:I:67:SER:HB3	3:I:406:HOH:O	1.99	0.62
1:J:25:ASN:H	1:J:27:LYS:HG3	1.64	0.62
1:P:352:SER:CA	3:P:501:HOH:O	2.47	0.62
1:Q:244:THR:HG23	1:Q:246:GLU:N	2.14	0.62
1:A:3:ARG:HD3	1:B:156:GLN:NE2	2.14	0.62
1:O:50:ASN:HD21	1:O:55:ARG:HH11	1.48	0.62
1:A:344:HIS:HB2	1:A:345:THR:O	2.00	0.62
1:E:244:THR:HG23	1:E:246:GLU:H	1.65	0.62
1:G:33:ASP:O	1:G:107:LYS:HE3	1.98	0.62
1:H:313:TRP:CZ2	1:H:315:GLY:HA2	2.34	0.62
1:H:66:ASP:O	1:H:67:SER:HB3	1.99	0.62
1:I:133:ARG:O	1:I:134:CYS:C	2.35	0.62
1:P:229:LYS:HG3	1:P:268:CYS:O	1.98	0.62
1:A:356:LEU:CD1	1:A:357:PHE:HE1	2.04	0.62
1:B:207:LYS:CD	1:C:2:HIS:HE2	2.12	0.62
1:B:58:PHE:CE1	1:B:310:LEU:CD1	2.78	0.62
1:D:67:SER:O	1:D:68:SER:C	2.33	0.62
1:J:244:THR:HG23	1:J:246:GLU:H	1.62	0.62
1:O:125:GLN:HE22	1:P:129:GLY:H	1.47	0.62
1:A:356:LEU:HD13	1:A:357:PHE:CD1	2.31	0.62
1:B:106:ILE:HG22	1:B:142:VAL:HG11	1.81	0.62
1:B:244:THR:O	1:B:247:GLN:N	2.32	0.62
1:I:130:LEU:O	1:I:134:CYS:N	2.25	0.62
1:M:51:THR:HG22	1:M:54:ASN:N	2.07	0.62
1:P:276:GLU:H	1:P:352:SER:HB3	1.64	0.62
1:D:81:GLU:HG2	1:D:82:THR:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:THR:CG2	1:I:247:GLN:H	2.13	0.62
1:J:3:ARG:O	1:J:4:PHE:C	2.36	0.62
1:N:51:THR:HG22	1:N:54:ASN:N	2.13	0.62
1:O:29:ILE:HB	1:O:300:SER:HA	1.81	0.62
1:P:123:THR:HG23	1:P:165:GLU:HG3	1.80	0.62
1:F:123:THR:CG2	1:F:165:GLU:HG3	2.30	0.62
1:M:67:SER:C	1:M:69:ILE:N	2.51	0.62
1:H:88:SER:O	1:H:89:GLN:HB2	2.00	0.62
1:I:125:GLN:NE2	1:J:129:GLY:H	1.98	0.62
1:R:271:SER:HA	1:R:274:MET:HE3	1.81	0.62
1:A:3:ARG:HD3	1:B:156:GLN:CD	2.21	0.62
1:H:220:HIS:HE1	3:H:407:HOH:O	1.81	0.62
1:H:58:PHE:CE1	1:H:310:LEU:HD13	2.35	0.62
1:G:187:GLU:HG3	1:G:229:LYS:HG2	1.82	0.62
1:L:69:ILE:HD13	1:L:73:ILE:HG12	1.82	0.62
1:O:148:ARG:HB2	1:O:187:GLU:OE1	2.00	0.62
1:C:202:GLN:HB2	1:C:233:VAL:HG11	1.81	0.61
1:D:336:GLN:HB2	1:D:342:TYR:HB2	1.82	0.61
1:L:17:GLU:O	1:L:21:SER:HB3	2.00	0.61
1:L:244:THR:HG22	1:L:247:GLN:CG	2.30	0.61
1:L:312:ALA:HB1	1:L:322:ALA:HB3	1.82	0.61
1:O:244:THR:N	1:O:247:GLN:OE1	2.32	0.61
1:E:87:ASP:O	1:E:89:GLN:HB3	1.99	0.61
1:F:276:GLU:CG	1:F:352:SER:HB3	2.30	0.61
1:G:119:ASN:O	1:G:152:ARG:NH1	2.31	0.61
1:J:244:THR:H	1:J:247:GLN:NE2	1.98	0.61
1:G:50:ASN:ND2	1:G:55:ARG:HH11	1.97	0.61
1:B:58:PHE:CZ	1:B:310:LEU:HD13	2.33	0.61
1:D:329:LYS:HD3	1:D:347:SER:H	1.65	0.61
1:O:118:THR:HA	1:P:1:ALA:H1	1.65	0.61
1:B:88:SER:O	1:B:89:GLN:HB2	2.00	0.61
1:E:89:GLN:N	3:E:504:HOH:O	2.34	0.61
1:G:51:THR:HG23	1:G:54:ASN:H	1.65	0.61
1:M:3:ARG:NH1	1:N:156:GLN:HE22	1.97	0.61
1:N:3:ARG:HB2	1:N:3:ARG:HH11	1.66	0.61
1:O:144:PHE:HA	1:O:183:VAL:H	1.64	0.61
1:P:58:PHE:CZ	1:P:310:LEU:HD13	2.35	0.61
1:B:80:HIS:CD2	1:B:137:TYR:OH	2.54	0.61
1:C:118:THR:HG21	1:C:121:GLU:HB2	1.81	0.61
1:E:244:THR:HG23	1:E:246:GLU:HB2	1.79	0.61
1:L:313:TRP:CZ2	1:L:315:GLY:HA2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:SER:HA	1:L:100:LYS:HD3	1.82	0.61
1:N:221:VAL:HG12	1:N:222:TYR:N	2.15	0.61
1:O:88:SER:O	1:O:89:GLN:HB2	1.98	0.61
1:Q:87:ASP:HB2	1:Q:91:LYS:O	2.01	0.61
1:R:244:THR:HG23	1:R:246:GLU:H	1.63	0.61
1:E:271:SER:O	1:E:274:MET:HE2	2.01	0.61
1:E:2:HIS:O	1:E:4:PHE:HD1	1.84	0.61
1:I:231:ASN:H	1:I:231:ASN:ND2	1.97	0.61
1:M:58:PHE:CE2	1:M:310:LEU:HD13	2.36	0.61
1:K:353:THR:CG2	1:O:92:LEU:HD11	2.31	0.61
1:P:276:GLU:HG3	1:P:352:SER:HB2	1.82	0.61
1:P:3:ARG:O	1:P:4:PHE:C	2.39	0.61
1:A:274:MET:HE3	1:A:279:ALA:HB2	1.81	0.61
1:A:156:GLN:NE2	1:B:3:ARG:HE	1.99	0.61
1:C:189:GLU:HG2	1:C:191:ILE:CD1	2.28	0.61
1:D:119:ASN:HB3	1:D:157:CYS:SG	2.41	0.61
1:F:195:ASP:HB3	1:F:238:ALA:HB3	1.83	0.61
1:O:182:LEU:N	1:O:182:LEU:HD23	2.15	0.61
1:R:124:ILE:HD13	3:R:514:HOH:O	2.01	0.61
1:R:58:PHE:CE1	1:R:310:LEU:HD13	2.36	0.61
1:E:1:ALA:N	1:E:220:HIS:HE1	1.98	0.61
1:K:12:LYS:HB3	1:K:222:TYR:CZ	2.36	0.61
1:A:202:GLN:HB2	1:A:233:VAL:HG11	1.83	0.61
1:M:272:GLY:HA2	1:M:303:ARG:NH1	2.16	0.61
1:R:276:GLU:HB3	1:R:330:ARG:HD3	1.82	0.61
1:R:95:ASN:O	1:R:99:GLU:HG3	2.00	0.61
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.36	0.60
1:B:78:LEU:O	1:B:106:ILE:HD12	2.01	0.60
1:F:80:HIS:CD2	1:F:137:TYR:OH	2.54	0.60
1:J:214:LYS:HG2	1:K:214:LYS:HG2	1.83	0.60
1:J:58:PHE:CE2	1:J:310:LEU:HD13	2.36	0.60
1:O:65:VAL:HG12	1:O:324:GLN:HB3	1.82	0.60
1:B:244:THR:HG22	1:B:247:GLN:CB	2.31	0.60
1:E:244:THR:HG21	1:E:246:GLU:HB2	1.82	0.60
1:I:123:THR:CG2	1:I:124:ILE:H	1.99	0.60
1:I:28:GLY:HA3	1:I:299:PHE:CZ	2.35	0.60
1:I:343:VAL:HG12	1:I:344:HIS:H	1.65	0.60
1:L:118:THR:HG22	1:L:121:GLU:H	1.61	0.60
1:M:345:THR:CB	3:M:502:HOH:O	2.49	0.60
1:R:271:SER:HA	1:R:274:MET:CE	2.31	0.60
1:R:313:TRP:CZ2	1:R:315:GLY:HA2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLU:HG2	1:D:191:ILE:HD11	1.79	0.60
1:E:118:THR:HG23	1:E:121:GLU:HG3	1.82	0.60
1:E:123:THR:HG23	1:E:165:GLU:HG3	1.83	0.60
1:E:233:VAL:HG23	1:E:252:THR:HA	1.83	0.60
1:F:276:GLU:HG3	1:F:352:SER:HB3	1.82	0.60
1:J:329:LYS:HZ2	1:J:347:SER:HA	1.65	0.60
1:K:156:GLN:HE22	1:L:3:ARG:NE	1.99	0.60
1:M:349:GLY:O	1:M:350:ALA:HB3	2.01	0.60
1:O:324:GLN:O	1:O:328:MET:HB3	2.01	0.60
1:B:123:THR:C	1:B:124:ILE:HD13	2.20	0.60
1:G:119:ASN:H	1:H:1:ALA:H1	1.48	0.60
1:H:250:MET:CE	1:H:291:LEU:HD22	2.31	0.60
1:M:1:ALA:H2	1:N:118:THR:HA	1.64	0.60
1:Q:344:HIS:ND1	1:Q:344:HIS:N	2.48	0.60
1:M:1:ALA:CB	1:N:119:ASN:H	2.12	0.60
1:N:3:ARG:CB	1:N:3:ARG:HH11	2.14	0.60
1:N:61:ILE:CG2	1:N:324:GLN:HG2	2.32	0.60
1:P:68:SER:O	1:P:71:GLN:HG3	2.01	0.60
1:R:8:THR:OG1	1:R:11:GLN:HG3	2.01	0.60
1:E:89:GLN:H	1:E:89:GLN:HE22	1.48	0.60
1:H:189:GLU:HG2	1:H:191:ILE:HD12	1.82	0.60
1:J:113:ALA:O	1:J:122:THR:HB	2.02	0.60
1:L:51:THR:HG22	1:L:54:ASN:CB	2.32	0.60
1:A:344:HIS:CG	1:A:344:HIS:O	2.54	0.60
1:C:232:MET:HG3	1:C:269:PHE:CD2	2.36	0.60
1:B:207:LYS:HD3	1:C:2:HIS:HE2	1.66	0.60
1:I:124:ILE:HG22	1:I:147:TRP:CZ2	2.37	0.60
1:K:91:LYS:HD3	1:K:96:ILE:HG12	1.84	0.60
1:Q:125:GLN:NE2	1:R:129:GLY:H	2.00	0.60
1:R:343:VAL:O	1:R:344:HIS:CG	2.54	0.60
1:A:91:LYS:HD3	1:A:96:ILE:HG12	1.83	0.60
1:I:274:MET:HE3	1:I:279:ALA:HA	1.84	0.60
1:J:352:SER:HA	3:J:503:HOH:O	2.01	0.60
1:L:12:LYS:HE2	1:L:222:TYR:CE1	2.37	0.60
1:O:277:GLU:OE2	1:O:342:TYR:OH	2.20	0.60
1:A:244:THR:HG23	1:A:246:GLU:N	2.17	0.60
1:A:45:ARG:NE	1:A:357:PHE:HA	2.17	0.60
1:B:61:ILE:CG2	1:B:323:THR:HG22	2.31	0.60
1:F:329:LYS:HD2	1:F:346:GLY:O	2.02	0.60
1:G:128:ASP:OD1	1:H:125:GLN:HB3	2.02	0.60
1:I:244:THR:HG22	1:I:247:GLN:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:343:VAL:O	1:L:344:HIS:ND1	2.35	0.60
1:M:65:VAL:HG12	1:M:68:SER:HB2	1.83	0.60
1:O:278:ASP:O	1:O:281:LEU:N	2.35	0.60
1:O:61:ILE:CG2	1:O:324:GLN:HG2	2.31	0.60
1:Q:109:ASP:HB2	1:Q:124:ILE:CG2	2.32	0.60
1:H:50:ASN:ND2	1:H:55:ARG:HD3	2.17	0.60
1:L:72:SER:HB3	1:L:331:ALA:O	2.02	0.60
1:N:313:TRP:CE2	1:N:315:GLY:CA	2.83	0.60
1:O:70:ASN:ND2	1:O:70:ASN:N	2.50	0.60
1:R:18:ILE:HD13	1:R:143:ASP:HB3	1.83	0.60
1:D:86:LYS:HD3	1:D:90:GLY:CA	2.31	0.59
1:L:272:GLY:HA2	1:L:303:ARG:NH1	2.17	0.59
1:L:91:LYS:HD3	1:L:96:ILE:CG1	2.32	0.59
1:M:80:HIS:HD2	1:M:137:TYR:OH	1.84	0.59
1:A:244:THR:CG2	1:A:247:GLN:N	2.46	0.59
1:C:50:ASN:HD21	1:C:55:ARG:HH11	1.48	0.59
1:F:33:ASP:HB3	1:F:77:ILE:HG22	1.84	0.59
1:I:271:SER:HB3	1:I:301:TYR:CE2	2.38	0.59
1:I:61:ILE:CG2	1:I:324:GLN:HG2	2.31	0.59
1:M:244:THR:HG23	1:M:247:GLN:OE1	2.01	0.59
1:Q:240:THR:O	1:Q:242:LYS:HE3	2.02	0.59
1:Q:330:ARG:HA	1:Q:330:ARG:HE	1.67	0.59
1:R:229:LYS:HA	1:R:268:CYS:O	2.02	0.59
1:C:118:THR:CG2	1:C:121:GLU:HB2	2.32	0.59
1:F:316:LYS:HB2	1:F:319:ASN:ND2	2.17	0.59
1:G:320:LYS:O	1:G:324:GLN:HG3	2.01	0.59
1:H:191:ILE:HD12	1:H:191:ILE:N	2.14	0.59
1:J:313:TRP:CE2	1:J:315:GLY:HA2	2.38	0.59
1:M:1:ALA:H3	1:N:119:ASN:H	1.50	0.59
1:N:123:THR:CG2	1:N:124:ILE:N	2.53	0.59
1:B:66:ASP:O	1:B:67:SER:O	2.21	0.59
1:E:276:GLU:HG3	1:E:352:SER:CB	2.32	0.59
1:E:51:THR:HG22	1:E:54:ASN:N	2.14	0.59
1:F:60:GLU:OE1	1:F:87:ASP:HB2	2.02	0.59
1:I:46:ILE:HG21	1:I:310:LEU:O	2.03	0.59
1:C:123:THR:HG22	1:C:124:ILE:N	2.11	0.59
1:D:63:PHE:O	1:D:100:LYS:HE3	2.01	0.59
1:F:352:SER:OG	1:F:356:LEU:HD11	2.02	0.59
1:M:2:HIS:NE2	1:P:207:LYS:HE2	2.17	0.59
1:C:58:PHE:CZ	1:C:310:LEU:HD13	2.37	0.59
1:F:51:THR:HG22	1:F:54:ASN:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:THR:HG22	1:G:247:GLN:N	2.18	0.59
1:H:313:TRP:CH2	1:H:315:GLY:HA2	2.37	0.59
1:I:29:ILE:HB	1:I:300:SER:HB2	1.85	0.59
1:K:303:ARG:NH2	1:K:357:PHE:CB	2.57	0.59
1:L:313:TRP:CE2	1:L:315:GLY:HA2	2.38	0.59
1:M:303:ARG:HD2	1:M:356:LEU:HB2	1.85	0.59
1:Q:170:LEU:HD22	1:Q:186:VAL:HG13	1.84	0.59
1:B:207:LYS:HZ3	1:C:2:HIS:HE2	1.49	0.59
1:D:190:VAL:H	1:D:231:ASN:ND2	2.00	0.59
1:H:115:LEU:O	1:H:118:THR:HB	2.03	0.59
1:I:58:PHE:CE2	1:I:62:LEU:HD11	2.36	0.59
1:J:12:LYS:O	1:J:13:LYS:C	2.41	0.59
1:J:224:GLU:OE1	1:J:224:GLU:N	2.31	0.59
1:L:123:THR:HG21	1:L:165:GLU:OE2	2.02	0.59
1:O:129:GLY:H	1:P:125:GLN:NE2	2.00	0.59
1:O:187:GLU:HG3	1:O:229:LYS:O	2.03	0.59
1:O:313:TRP:CZ2	1:O:315:GLY:HA2	2.38	0.59
1:P:313:TRP:CD2	1:P:315:GLY:HA2	2.38	0.59
1:C:12:LYS:HG2	1:C:222:TYR:CE1	2.37	0.59
1:H:281:LEU:HD22	1:H:344:HIS:CE1	2.37	0.59
1:N:343:VAL:O	1:N:344:HIS:C	2.38	0.59
1:B:2:HIS:O	1:B:2:HIS:CD2	2.55	0.59
1:B:29:ILE:HB	1:B:300:SER:HA	1.84	0.59
1:H:299:PHE:CD1	1:H:334:ASN:HB3	2.37	0.59
1:J:28:GLY:HA3	1:J:299:PHE:CZ	2.38	0.59
1:J:42:ARG:CG	1:J:42:ARG:HH11	2.14	0.59
1:O:65:VAL:HG21	1:O:328:MET:HE2	1.84	0.59
1:R:124:ILE:CG2	1:R:147:TRP:CE2	2.86	0.59
1:C:344:HIS:O	1:C:345:THR:C	2.41	0.59
1:D:1:ALA:HB1	1:D:2:HIS:ND1	2.17	0.59
1:G:188:PRO:O	1:G:188:PRO:CG	2.45	0.59
1:G:330:ARG:HE	1:G:330:ARG:HA	1.66	0.59
1:B:343:VAL:O	1:B:343:VAL:HG22	2.02	0.58
1:B:58:PHE:CE2	1:B:62:LEU:HD21	2.37	0.58
1:B:66:ASP:O	1:B:67:SER:C	2.41	0.58
1:C:156:GLN:HE22	1:D:3:ARG:HD2	1.65	0.58
1:F:271:SER:O	1:F:274:MET:HB2	2.03	0.58
1:H:118:THR:HG23	1:H:121:GLU:H	1.66	0.58
1:I:258:ARG:NH1	1:L:224:GLU:OE2	2.32	0.58
1:N:63:PHE:HB3	1:N:97:LEU:HD21	1.85	0.58
1:Q:244:THR:HG22	1:Q:247:GLN:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:O	1:B:218:ASP:HB2	2.03	0.58
1:E:223:LEU:O	1:E:226:THR:HB	2.03	0.58
1:L:18:ILE:HD13	1:L:143:ASP:HB3	1.85	0.58
1:N:108:LEU:HD12	1:N:173:TYR:HE1	1.68	0.58
1:M:1:ALA:HB1	1:N:156:GLN:HB3	1.85	0.58
1:Q:271:SER:HA	1:Q:274:MET:CE	2.33	0.58
1:A:125:GLN:NE2	1:B:129:GLY:H	1.94	0.58
1:G:12:LYS:HB3	1:G:222:TYR:CZ	2.38	0.58
1:G:3:ARG:CG	1:G:3:ARG:HH11	2.16	0.58
1:J:123:THR:HG21	1:J:165:GLU:OE2	2.03	0.58
1:M:3:ARG:HG3	1:M:4:PHE:H	1.68	0.58
1:N:58:PHE:CE1	1:N:310:LEU:CD1	2.86	0.58
1:O:118:THR:HG21	1:O:121:GLU:HB2	1.84	0.58
1:P:146:LYS:HE2	1:P:187:GLU:OE1	2.04	0.58
1:D:329:LYS:HZ2	1:D:347:SER:HA	1.67	0.58
1:D:343:VAL:HG12	1:D:344:HIS:N	2.19	0.58
1:I:198:LEU:CD1	1:I:234:THR:HA	2.34	0.58
1:I:250:MET:HE3	1:I:291:LEU:HD21	1.85	0.58
1:I:2:HIS:CB	1:J:156:GLN:OE1	2.52	0.58
1:G:29:ILE:HB	1:G:300:SER:HA	1.84	0.58
1:L:244:THR:N	1:L:247:GLN:OE1	2.36	0.58
1:Q:161:LEU:HB3	3:Q:2023:HOH:O	2.01	0.58
1:C:2:HIS:CB	1:D:156:GLN:OE1	2.51	0.58
1:F:271:SER:HA	1:F:274:MET:HE2	1.84	0.58
1:M:3:ARG:HG2	1:M:4:PHE:CD1	2.39	0.58
1:M:69:ILE:HG22	1:M:71:GLN:HG2	1.84	0.58
1:O:123:THR:HG21	1:O:165:GLU:OE2	2.04	0.58
1:R:118:THR:HG23	1:R:121:GLU:HG3	1.84	0.58
1:A:307:ALA:HB2	1:A:357:PHE:CE1	2.38	0.58
1:D:278:ASP:O	1:D:279:ALA:C	2.42	0.58
1:E:88:SER:C	1:E:89:GLN:CD	2.62	0.58
1:F:50:ASN:ND2	1:F:55:ARG:HD3	2.19	0.58
1:L:281:LEU:CD2	1:L:342:TYR:HE2	2.14	0.58
1:N:253:VAL:O	1:N:257:HIS:HB3	2.03	0.58
1:O:51:THR:CG2	1:O:54:ASN:N	2.65	0.58
1:Q:202:GLN:HB2	1:Q:233:VAL:HG11	1.85	0.58
1:Q:91:LYS:NZ	1:Q:99:GLU:OE1	2.36	0.58
1:A:2:HIS:C	1:A:4:PHE:H	2.03	0.58
1:B:223:LEU:O	1:B:226:THR:HB	2.04	0.58
1:B:344:HIS:C	1:B:345:THR:O	2.40	0.58
1:B:207:LYS:HZ3	1:C:2:HIS:CD2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:HG23	1:C:53:GLU:N	2.19	0.58
1:E:89:GLN:CA	3:E:504:HOH:O	2.51	0.58
1:G:322:ALA:O	1:G:325:GLU:N	2.36	0.58
1:H:330:ARG:NH1	1:H:347:SER:HB3	2.19	0.58
1:I:138:LYS:HD2	3:I:412:HOH:O	2.02	0.58
1:K:87:ASP:OD2	1:K:89:GLN:HB2	2.04	0.58
1:M:69:ILE:C	1:M:71:GLN:N	2.55	0.58
1:N:68:SER:O	1:N:69:ILE:C	2.42	0.58
1:O:128:ASP:HB2	1:P:128:ASP:OD2	2.03	0.58
1:P:50:ASN:HD21	1:P:55:ARG:HH11	1.49	0.58
1:B:51:THR:CG2	1:B:54:ASN:HB2	2.22	0.58
1:H:118:THR:HG23	1:H:121:GLU:HG3	1.85	0.58
1:I:51:THR:HB	1:I:54:ASN:HB2	1.86	0.58
1:K:177:CYS:HB3	1:K:182:LEU:HB2	1.86	0.58
1:K:51:THR:CG2	1:K:54:ASN:N	2.63	0.58
1:D:61:ILE:HG21	1:D:323:THR:CG2	2.33	0.57
1:K:118:THR:CG2	1:K:121:GLU:H	2.16	0.57
1:K:237:HIS:NE2	1:K:357:PHE:O	2.37	0.57
1:A:291:LEU:O	1:A:293:LYS:HG3	2.05	0.57
1:F:233:VAL:HG23	1:F:252:THR:HA	1.86	0.57
1:G:58:PHE:CE2	1:G:62:LEU:HD11	2.38	0.57
1:O:123:THR:CG2	1:O:165:GLU:HG3	2.34	0.57
1:A:277:GLU:HG2	1:A:347:SER:HB3	1.86	0.57
1:A:303:ARG:CB	1:A:357:PHE:CD1	2.87	0.57
1:C:12:LYS:HG2	1:C:222:TYR:CZ	2.39	0.57
1:K:80:HIS:CD2	1:K:137:TYR:OH	2.53	0.57
1:Q:118:THR:CG2	1:Q:121:GLU:H	2.17	0.57
1:B:151:LEU:HD12	1:B:208:VAL:HG11	1.86	0.57
1:E:347:SER:OG	1:E:348:SER:N	2.36	0.57
1:F:291:LEU:O	1:F:293:LYS:HG3	2.04	0.57
1:I:183:VAL:HG12	1:I:183:VAL:O	2.02	0.57
1:M:159:SER:O	1:M:163:ILE:HG13	2.04	0.57
1:M:224:GLU:OE1	1:M:224:GLU:N	2.34	0.57
1:P:118:THR:CG2	1:P:121:GLU:HB2	2.33	0.57
1:P:155:ASP:OD1	1:P:156:GLN:HG3	2.05	0.57
1:C:150:VAL:HG13	1:C:191:ILE:HG12	1.86	0.57
1:B:207:LYS:HD3	1:C:2:HIS:NE2	2.19	0.57
1:I:284:ASN:OD1	1:I:340:GLY:HA2	2.05	0.57
1:L:219:HIS:O	1:L:220:HIS:HB2	2.04	0.57
1:P:77:ILE:HD13	1:P:146:LYS:HG3	1.86	0.57
1:H:9:GLN:HA	1:H:9:GLN:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:309:ALA:HB1	1:R:323:THR:CG2	2.33	0.57
1:B:248:VAL:O	1:B:249:ALA:C	2.42	0.57
1:B:298:SER:OG	1:B:299:PHE:N	2.34	0.57
1:B:343:VAL:O	1:B:344:HIS:C	2.42	0.57
1:C:147:TRP:HB2	1:C:173:TYR:CZ	2.40	0.57
1:G:319:ASN:O	1:G:320:LYS:C	2.42	0.57
1:I:118:THR:HG23	1:I:121:GLU:H	1.67	0.57
1:L:91:LYS:HD3	1:L:96:ILE:HG12	1.86	0.57
1:M:235:ALA:HB2	1:M:243:TYR:CE1	2.40	0.57
1:M:329:LYS:NZ	1:M:348:SER:HB2	2.20	0.57
1:A:44:GLN:HA	1:A:44:GLN:OE1	2.04	0.57
1:E:203:TYR:OH	1:H:2:HIS:HA	2.03	0.57
1:G:119:ASN:N	1:H:1:ALA:H3	1.97	0.57
1:I:80:HIS:HD2	1:I:137:TYR:OH	1.88	0.57
1:N:18:ILE:HD13	1:N:143:ASP:HB3	1.86	0.57
1:J:50:ASN:ND2	1:J:55:ARG:HH11	2.03	0.57
1:M:106:ILE:O	1:M:106:ILE:HG23	2.04	0.57
1:M:71:GLN:NE2	3:M:501:HOH:O	1.63	0.57
1:O:230:PRO:HG3	1:O:267:ILE:HD13	1.85	0.57
1:P:8:THR:N	1:P:11:GLN:OE1	2.34	0.57
1:I:68:SER:HA	1:I:70:ASN:HD21	1.67	0.57
1:M:244:THR:HG23	1:M:247:GLN:CG	2.33	0.57
1:N:271:SER:O	1:N:272:GLY:C	2.40	0.57
1:B:123:THR:HG21	1:B:165:GLU:OE2	2.04	0.56
1:B:155:ASP:O	1:B:156:GLN:HB2	2.04	0.56
1:G:219:HIS:O	1:G:220:HIS:HB2	2.05	0.56
1:I:319:ASN:O	1:I:320:LYS:C	2.43	0.56
1:L:220:HIS:CE1	3:L:407:HOH:O	2.53	0.56
1:L:335:CYS:O	1:L:339:LYS:HD2	2.05	0.56
1:A:126:GLY:N	1:B:128:ASP:OD1	2.37	0.56
1:B:244:THR:HG23	1:B:246:GLU:N	2.20	0.56
1:C:2:HIS:O	1:D:156:GLN:OE1	2.23	0.56
1:I:2:HIS:O	1:I:3:ARG:C	2.43	0.56
1:J:214:LYS:CG	1:K:214:LYS:HG2	2.36	0.56
1:M:313:TRP:O	1:M:315:GLY:N	2.38	0.56
1:N:2:HIS:CA	1:N:3:ARG:NH1	2.68	0.56
1:O:156:GLN:OE1	1:P:2:HIS:CB	2.49	0.56
1:D:70:ASN:CB	1:D:71:GLN:N	2.67	0.56
1:G:244:THR:HG22	1:G:247:GLN:HG3	1.88	0.56
1:G:276:GLU:HB3	1:G:330:ARG:HH11	1.70	0.56
1:K:244:THR:HG23	1:K:246:GLU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:LEU:O	1:L:226:THR:HB	2.05	0.56
1:O:244:THR:O	1:O:247:GLN:N	2.39	0.56
1:Q:244:THR:HG22	1:Q:247:GLN:HG3	1.88	0.56
1:B:87:ASP:O	1:B:88:SER:HB2	2.06	0.56
1:E:244:THR:HG22	1:E:247:GLN:HG3	1.87	0.56
1:F:244:THR:HG23	1:F:247:GLN:H	1.69	0.56
1:F:58:PHE:CE1	1:F:310:LEU:HD13	2.40	0.56
1:J:118:THR:HG23	1:J:121:GLU:H	1.70	0.56
1:M:306:GLN:O	1:M:310:LEU:HB2	2.04	0.56
1:M:329:LYS:HZ1	1:M:348:SER:HB2	1.70	0.56
1:N:313:TRP:CH2	1:N:315:GLY:HA2	2.39	0.56
1:O:244:THR:HG23	1:O:246:GLU:N	2.19	0.56
1:O:330:ARG:HA	1:O:330:ARG:NE	2.19	0.56
1:C:271:SER:HB3	1:C:301:TYR:CD2	2.39	0.56
1:E:50:ASN:ND2	1:E:55:ARG:HD3	2.20	0.56
1:G:3:ARG:CD	1:H:156:GLN:HE22	2.18	0.56
1:I:50:ASN:HD21	1:I:55:ARG:HH11	1.52	0.56
1:P:118:THR:HG21	1:P:121:GLU:HB2	1.88	0.56
1:C:46:ILE:HG13	1:C:48:VAL:HG23	1.87	0.56
1:D:329:LYS:CE	1:D:347:SER:N	2.69	0.56
1:D:330:ARG:HA	1:D:330:ARG:NE	2.19	0.56
1:H:250:MET:CE	1:H:291:LEU:CD2	2.83	0.56
1:I:244:THR:HG22	1:I:247:GLN:CB	2.35	0.56
1:L:44:GLN:HA	1:L:44:GLN:OE1	2.06	0.56
1:M:118:THR:HG23	1:M:121:GLU:N	2.13	0.56
1:M:308:SER:CB	1:M:351:ALA:HB1	2.32	0.56
1:O:1:ALA:HB1	1:P:159:SER:HB3	1.87	0.56
1:P:276:GLU:CB	1:P:352:SER:HB3	2.36	0.56
1:Q:244:THR:HG22	1:Q:247:GLN:H	1.71	0.56
1:A:154:ALA:HB3	1:A:157:CYS:CB	2.33	0.56
1:E:233:VAL:CG2	1:E:252:THR:HA	2.36	0.56
1:E:88:SER:CA	1:E:89:GLN:HB3	2.12	0.56
1:F:190:VAL:H	1:F:231:ASN:HD22	1.54	0.56
1:G:51:THR:HG22	1:G:54:ASN:HB2	1.88	0.56
1:I:272:GLY:HA2	1:I:303:ARG:NH1	2.21	0.56
1:J:352:SER:CB	3:J:503:HOH:O	2.53	0.56
1:Q:115:LEU:O	1:Q:118:THR:HB	2.05	0.56
1:D:313:TRP:CE2	1:D:315:GLY:HA2	2.41	0.56
1:D:277:GLU:OE2	1:D:344:HIS:ND1	2.38	0.56
1:I:118:THR:CG2	1:I:121:GLU:N	2.66	0.56
1:I:244:THR:HG22	1:I:247:GLN:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:308:SER:O	1:O:311:ALA:HB3	2.06	0.56
1:R:344:HIS:HD2	3:R:566:HOH:O	1.88	0.56
1:B:281:LEU:CD2	1:B:344:HIS:ND1	2.62	0.56
1:B:66:ASP:OD1	1:B:67:SER:N	2.39	0.56
1:B:89:GLN:O	1:B:90:GLY:C	2.39	0.56
1:O:118:THR:CG2	1:O:121:GLU:H	2.19	0.56
1:O:168:ASN:HB3	3:P:504:HOH:O	2.05	0.56
1:P:12:LYS:HD3	1:P:222:TYR:CE1	2.41	0.56
1:D:187:GLU:HG3	1:D:229:LYS:HB3	1.88	0.56
1:D:329:LYS:HD3	1:D:347:SER:CA	2.35	0.56
1:E:271:SER:O	1:E:274:MET:CE	2.54	0.56
1:H:78:LEU:O	1:H:106:ILE:HD12	2.06	0.56
1:I:198:LEU:HD12	1:I:234:THR:HA	1.87	0.56
1:I:250:MET:CE	1:I:291:LEU:HD21	2.36	0.56
1:J:230:PRO:CG	1:J:267:ILE:HD12	2.31	0.56
1:J:352:SER:HB2	3:J:503:HOH:O	2.04	0.56
1:I:200:HIS:CE1	1:L:2:HIS:ND1	2.65	0.56
1:M:68:SER:CB	1:M:69:ILE:CD1	2.77	0.56
1:P:333:ALA:HB1	1:P:342:TYR:CE1	2.41	0.56
1:C:147:TRP:HB3	1:C:173:TYR:CE2	2.41	0.56
1:I:200:HIS:HE1	1:L:2:HIS:CE1	2.23	0.56
1:I:324:GLN:O	1:I:328:MET:HB2	2.05	0.56
1:J:329:LYS:HD3	1:J:347:SER:N	2.20	0.56
1:M:6:ALA:O	1:M:7:LEU:HD23	2.06	0.56
1:P:28:GLY:HA3	1:P:299:PHE:CE1	2.40	0.56
1:R:190:VAL:H	1:R:231:ASN:HD22	1.53	0.56
1:D:329:LYS:HD3	1:D:347:SER:HB2	1.87	0.55
1:F:200:HIS:HB2	3:F:467:HOH:O	2.06	0.55
1:F:344:HIS:CG	1:F:345:THR:N	2.73	0.55
1:G:128:ASP:HA	1:H:125:GLN:HE21	1.72	0.55
1:H:18:ILE:HD13	1:H:143:ASP:HB3	1.88	0.55
1:I:66:ASP:O	1:I:67:SER:CB	2.50	0.55
1:K:8:THR:OG1	1:K:11:GLN:HG3	2.06	0.55
1:L:244:THR:CG2	1:L:247:GLN:N	2.61	0.55
1:O:58:PHE:CZ	1:O:62:LEU:HD21	2.41	0.55
1:A:342:TYR:CZ	1:A:344:HIS:HB3	2.39	0.55
1:A:303:ARG:HH21	1:A:359:ALA:CB	2.18	0.55
1:A:51:THR:CG2	1:A:53:GLU:N	2.69	0.55
1:B:124:ILE:HG22	1:B:147:TRP:CZ2	2.41	0.55
1:F:244:THR:HG22	1:F:247:GLN:CB	2.35	0.55
1:G:65:VAL:HG12	1:G:324:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:ASP:O	1:H:67:SER:CB	2.54	0.55
1:I:123:THR:CG2	1:I:124:ILE:N	2.64	0.55
1:M:119:ASN:HB2	1:N:4:PHE:CZ	2.41	0.55
1:O:1:ALA:N	1:P:118:THR:HA	2.21	0.55
1:P:276:GLU:N	1:P:352:SER:HB3	2.21	0.55
1:R:244:THR:HG23	1:R:246:GLU:HB2	1.88	0.55
1:B:151:LEU:CD1	1:B:208:VAL:HG11	2.37	0.55
1:C:322:ALA:O	1:C:325:GLU:HB2	2.06	0.55
1:F:329:LYS:HE2	1:F:347:SER:CA	2.05	0.55
1:I:29:ILE:HB	1:I:300:SER:HA	1.87	0.55
1:I:58:PHE:CE1	1:I:310:LEU:HD13	2.41	0.55
1:O:281:LEU:HD23	1:O:342:TYR:HE2	1.70	0.55
1:M:2:HIS:CE1	1:P:203:TYR:HH	2.20	0.55
1:P:226:THR:HG23	3:P:520:HOH:O	2.00	0.55
1:A:303:ARG:HB3	1:A:357:PHE:CE1	2.41	0.55
1:E:3:ARG:O	1:E:3:ARG:HD2	2.07	0.55
1:J:214:LYS:HE3	1:J:218:ASP:OD1	2.06	0.55
1:M:1:ALA:H2	1:N:118:THR:CA	2.14	0.55
1:A:123:THR:HG22	1:A:124:ILE:H	1.72	0.55
1:H:253:VAL:CG1	1:H:291:LEU:HD23	2.35	0.55
1:I:244:THR:HG22	1:I:247:GLN:CG	2.36	0.55
1:L:118:THR:HG21	1:L:121:GLU:HB2	1.87	0.55
1:M:221:VAL:HG12	1:M:222:TYR:N	2.22	0.55
1:B:342:TYR:O	1:B:344:HIS:N	2.39	0.55
1:C:124:ILE:HG22	1:C:147:TRP:CZ2	2.42	0.55
1:C:2:HIS:CD2	1:C:3:ARG:HH11	2.25	0.55
1:J:272:GLY:HA2	1:J:303:ARG:NH1	2.22	0.55
1:K:347:SER:O	1:O:90:GLY:HA3	2.07	0.55
1:M:1:ALA:HB3	1:N:119:ASN:HB3	1.89	0.55
1:O:203:TYR:C	1:O:203:TYR:CD2	2.79	0.55
1:O:278:ASP:O	1:O:279:ALA:C	2.45	0.55
1:B:123:THR:CG2	1:B:165:GLU:HG3	2.30	0.55
1:B:22:ILE:O	1:B:22:ILE:HG22	2.06	0.55
1:H:59:ARG:HB3	1:H:63:PHE:CE1	2.42	0.55
1:J:123:THR:HG23	1:J:165:GLU:HG3	1.89	0.55
1:M:1:ALA:HB3	1:N:119:ASN:N	2.13	0.55
1:M:320:LYS:O	1:M:324:GLN:HG3	2.07	0.55
1:M:65:VAL:HG13	1:M:328:MET:SD	2.47	0.55
1:O:204:VAL:O	1:O:208:VAL:HG23	2.07	0.55
1:E:89:GLN:HA	3:E:504:HOH:O	2.07	0.55
1:F:124:ILE:HG22	1:F:147:TRP:CZ2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ASN:HD21	1:G:55:ARG:HH11	1.54	0.55
1:I:128:ASP:OD1	1:J:125:GLN:HB3	2.06	0.55
1:K:115:LEU:HD13	1:K:123:THR:OG1	2.07	0.55
1:Q:159:SER:HB3	1:R:1:ALA:N	2.19	0.55
1:A:51:THR:HG23	1:A:53:GLU:H	1.71	0.55
1:H:320:LYS:O	1:H:324:GLN:HG3	2.06	0.55
1:K:120:LYS:HB2	1:K:152:ARG:HH12	1.72	0.55
1:K:150:VAL:HG13	1:K:191:ILE:HG13	1.89	0.55
1:K:357:PHE:C	1:O:139:LYS:HZ2	2.11	0.55
1:M:3:ARG:O	1:M:4:PHE:C	2.45	0.55
1:D:277:GLU:OE2	1:D:344:HIS:CE1	2.60	0.55
1:G:229:LYS:HA	1:G:268:CYS:O	2.07	0.55
1:G:28:GLY:HA3	1:G:299:PHE:CE1	2.41	0.55
1:H:339:LYS:NZ	3:H:403:HOH:O	2.40	0.55
1:I:156:GLN:HE22	1:J:3:ARG:HG3	1.72	0.55
1:J:71:GLN:NE2	3:J:504:HOH:O	2.39	0.55
1:K:156:GLN:OE1	1:L:2:HIS:N	2.36	0.55
1:L:229:LYS:HA	1:L:268:CYS:O	2.07	0.55
1:M:150:VAL:HG13	1:M:191:ILE:HG12	1.89	0.55
1:L:187:GLU:HG3	1:L:229:LYS:O	2.08	0.54
1:L:256:LEU:O	1:L:257:HIS:C	2.45	0.54
1:M:65:VAL:CG1	1:M:68:SER:HB2	2.37	0.54
1:N:58:PHE:CE1	1:N:310:LEU:HD13	2.42	0.54
1:O:118:THR:HA	1:P:1:ALA:H3	1.72	0.54
1:D:1:ALA:CB	1:D:2:HIS:ND1	2.70	0.54
1:E:2:HIS:O	1:F:156:GLN:OE1	2.25	0.54
1:I:121:GLU:OE1	1:I:159:SER:HB3	2.07	0.54
1:N:115:LEU:HD13	1:N:123:THR:OG1	2.07	0.54
1:O:223:LEU:O	1:O:226:THR:HB	2.06	0.54
1:C:58:PHE:CE1	1:C:310:LEU:HD13	2.42	0.54
1:C:125:GLN:HE21	1:D:129:GLY:H	1.55	0.54
1:F:123:THR:C	1:F:124:ILE:HD12	2.28	0.54
1:H:277:GLU:OE2	1:H:345:THR:HA	2.07	0.54
1:I:149:ALA:HB1	1:I:166:ASN:OD1	2.07	0.54
1:M:159:SER:CB	1:N:1:ALA:HA	2.37	0.54
1:O:51:THR:HG23	1:O:54:ASN:H	1.71	0.54
1:C:244:THR:HG23	1:C:246:GLU:N	2.22	0.54
1:C:271:SER:O	1:C:272:GLY:C	2.46	0.54
1:E:8:THR:O	1:E:12:LYS:HG3	2.07	0.54
1:G:51:THR:HG22	1:G:54:ASN:CB	2.37	0.54
1:H:86:LYS:CB	1:H:90:GLY:HA2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:320:LYS:O	1:N:324:GLN:HG3	2.07	0.54
1:O:148:ARG:NH1	1:O:189:GLU:OE1	2.37	0.54
1:D:329:LYS:CD	1:D:347:SER:H	2.21	0.54
1:F:256:LEU:HD13	1:F:267:ILE:CD1	2.37	0.54
1:J:83:LEU:HG	1:J:83:LEU:O	2.08	0.54
1:M:124:ILE:HG21	1:M:147:TRP:NE1	2.22	0.54
1:B:207:LYS:NZ	1:C:2:HIS:HE2	2.06	0.54
1:E:219:HIS:O	1:E:220:HIS:HB2	2.08	0.54
1:I:171:ALA:HA	1:I:216:LEU:HD12	1.88	0.54
1:I:244:THR:HG22	1:I:247:GLN:HG3	1.90	0.54
1:I:65:VAL:CG1	1:I:69:ILE:HG21	2.38	0.54
1:L:149:ALA:HB3	1:L:188:PRO:HA	1.90	0.54
1:L:233:VAL:O	1:L:248:VAL:HG13	2.07	0.54
1:M:117:GLY:O	1:N:3:ARG:HD3	2.07	0.54
1:O:271:SER:HA	1:O:274:MET:HE2	1.90	0.54
1:R:29:ILE:HB	1:R:300:SER:HA	1.90	0.54
1:I:271:SER:HB2	1:I:274:MET:HE2	1.90	0.54
1:K:221:VAL:HG12	1:K:222:TYR:N	2.21	0.54
1:L:312:ALA:HB1	1:L:322:ALA:CB	2.38	0.54
1:M:303:ARG:HG3	1:M:303:ARG:HH11	1.72	0.54
1:B:146:LYS:HE2	1:B:187:GLU:OE1	2.07	0.54
1:D:329:LYS:HD3	1:D:347:SER:N	2.22	0.54
1:M:226:THR:HG23	3:M:509:HOH:O	2.08	0.54
1:M:1:ALA:N	1:N:118:THR:OG1	2.40	0.54
1:P:91:LYS:HD3	1:P:96:ILE:HG12	1.90	0.54
1:D:313:TRP:CZ2	1:D:315:GLY:HA2	2.42	0.54
1:M:4:PHE:CZ	1:N:119:ASN:HB2	2.42	0.54
1:N:276:GLU:HB3	1:N:330:ARG:NH1	2.23	0.54
1:Q:233:VAL:HG23	1:Q:252:THR:HA	1.89	0.54
1:R:271:SER:HB3	1:R:301:TYR:CD2	2.42	0.54
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.43	0.54
1:B:202:GLN:O	1:B:206:GLU:N	2.36	0.54
1:H:63:PHE:O	1:H:100:LYS:NZ	2.41	0.54
1:I:190:VAL:H	1:I:231:ASN:HD22	1.55	0.54
1:I:330:ARG:NE	1:I:330:ARG:HA	2.20	0.54
1:J:226:THR:HG23	3:J:511:HOH:O	2.08	0.54
1:B:29:ILE:HB	1:B:300:SER:CB	2.37	0.53
1:C:197:ASP:C	1:C:197:ASP:OD1	2.46	0.53
1:C:313:TRP:CE2	1:C:315:GLY:CA	2.88	0.53
1:C:3:ARG:HD3	1:C:3:ARG:N	2.22	0.53
1:C:53:GLU:OE1	1:C:53:GLU:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:THR:HG22	1:F:247:GLN:H	1.73	0.53
1:L:42:ARG:O	1:L:45:ARG:HB2	2.08	0.53
1:Q:22:ILE:HD11	1:Q:144:PHE:CD2	2.43	0.53
1:R:271:SER:CA	1:R:274:MET:HE3	2.38	0.53
1:B:319:ASN:O	1:B:320:LYS:C	2.45	0.53
1:C:1:ALA:CB	1:C:4:PHE:CD1	2.92	0.53
1:C:244:THR:HG23	1:C:247:GLN:N	2.23	0.53
1:E:195:ASP:O	1:E:239:CYS:HB2	2.06	0.53
1:E:351:ALA:O	1:E:352:SER:CB	2.50	0.53
1:E:8:THR:HG23	1:E:11:GLN:OE1	2.07	0.53
1:F:189:GLU:HG2	1:F:191:ILE:HD13	1.89	0.53
1:F:71:GLN:CG	3:F:401:HOH:O	2.31	0.53
1:G:291:LEU:O	1:G:293:LYS:HG3	2.08	0.53
1:J:190:VAL:H	1:J:231:ASN:ND2	2.04	0.53
1:J:342:TYR:OH	1:J:345:THR:N	2.41	0.53
1:M:279:ALA:HB1	1:M:301:TYR:CE1	2.43	0.53
1:N:2:HIS:C	1:N:3:ARG:NH1	2.61	0.53
1:N:51:THR:O	1:N:52:GLU:C	2.45	0.53
1:O:313:TRP:CE2	1:O:315:GLY:HA2	2.43	0.53
1:B:115:LEU:O	1:B:118:THR:HB	2.08	0.53
1:C:271:SER:HA	1:C:274:MET:HE2	1.90	0.53
1:G:267:ILE:HG12	1:G:297:LEU:HD23	1.91	0.53
1:H:124:ILE:CD1	3:H:426:HOH:O	2.56	0.53
1:H:329:LYS:HD2	1:H:347:SER:CB	2.38	0.53
1:H:276:GLU:H	1:H:352:SER:CB	2.22	0.53
1:I:277:GLU:HG3	1:I:281:LEU:HD11	1.91	0.53
1:J:2:HIS:O	1:J:3:ARG:O	2.26	0.53
1:M:1:ALA:H3	1:N:118:THR:C	2.11	0.53
1:N:224:GLU:OE2	1:O:258:ARG:HD3	2.09	0.53
1:A:244:THR:HG23	1:A:246:GLU:H	1.71	0.53
1:C:128:ASP:OD1	1:D:126:GLY:N	2.40	0.53
1:D:91:LYS:HG2	1:D:96:ILE:HG13	1.90	0.53
1:K:206:GLU:HG2	1:K:255:ALA:HA	1.90	0.53
1:L:13:LYS:O	1:L:17:GLU:HG3	2.08	0.53
1:M:329:LYS:NZ	1:M:347:SER:C	2.61	0.53
1:A:95:ASN:O	1:A:99:GLU:HG3	2.09	0.53
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.91	0.53
1:D:67:SER:O	1:D:69:ILE:N	2.42	0.53
1:E:91:LYS:HD3	1:E:96:ILE:HG12	1.90	0.53
1:J:348:SER:OG	1:J:349:GLY:N	2.41	0.53
1:M:25:ASN:H	1:M:27:LYS:HG3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:123:THR:CG2	1:P:124:ILE:H	2.12	0.53
1:B:245:PRO:HA	1:B:282:ASN:OD1	2.08	0.53
1:B:341:GLN:O	1:B:342:TYR:C	2.47	0.53
1:C:115:LEU:O	1:C:118:THR:HB	2.09	0.53
1:C:2:HIS:CD2	1:C:3:ARG:NH1	2.76	0.53
1:E:349:GLY:O	1:E:351:ALA:N	2.42	0.53
1:F:330:ARG:HE	1:F:347:SER:HB2	1.74	0.53
1:H:123:THR:HG23	1:H:165:GLU:HG3	1.91	0.53
1:H:354:GLN:HG2	1:H:356:LEU:HD21	1.89	0.53
1:L:244:THR:O	1:L:244:THR:CG2	2.56	0.53
1:P:345:THR:HG22	1:P:346:GLY:N	2.23	0.53
1:R:50:ASN:ND2	1:R:55:ARG:HH11	2.07	0.53
1:B:17:GLU:O	1:B:18:ILE:C	2.45	0.53
1:E:172:ARG:NH2	1:E:176:ILE:HD11	2.23	0.53
1:G:313:TRP:CD2	1:G:315:GLY:HA2	2.43	0.53
1:I:274:MET:HE3	1:I:279:ALA:CA	2.38	0.53
1:I:66:ASP:O	1:I:67:SER:HB3	2.07	0.53
1:J:160:SER:O	1:J:164:GLN:HB3	2.08	0.53
1:K:357:PHE:C	1:O:139:LYS:HE3	2.29	0.53
1:M:124:ILE:HG22	1:M:147:TRP:CZ2	2.44	0.53
1:P:354:GLN:O	1:P:355:SER:CB	2.56	0.53
1:Q:276:GLU:HB3	1:Q:330:ARG:HD3	1.90	0.53
1:R:198:LEU:CD1	1:R:234:THR:HA	2.39	0.53
1:R:214:LYS:HD2	1:R:214:LYS:C	2.29	0.53
1:A:294:PRO:HG2	1:A:295:TRP:CE2	2.43	0.53
1:B:228:LEU:O	1:B:267:ILE:HA	2.09	0.53
1:B:65:VAL:CG2	1:B:324:GLN:HB3	2.39	0.53
1:E:68:SER:O	1:E:71:GLN:HB2	2.09	0.53
1:H:68:SER:O	1:H:71:GLN:HB2	2.09	0.53
1:I:41:ASN:O	1:I:44:GLN:HB3	2.08	0.53
1:J:199:GLU:HB2	3:J:534:HOH:O	2.09	0.53
1:K:22:ILE:O	1:K:22:ILE:HG22	2.08	0.53
1:M:253:VAL:O	1:M:254:THR:C	2.43	0.53
1:Q:291:LEU:O	1:Q:293:LYS:HG3	2.09	0.53
1:R:121:GLU:OE1	1:R:159:SER:HB3	2.09	0.53
1:R:87:ASP:O	1:R:89:GLN:N	2.36	0.53
1:C:244:THR:CG2	1:C:244:THR:O	2.57	0.53
1:D:189:GLU:CG	1:D:191:ILE:HD11	2.38	0.53
1:E:271:SER:CA	1:E:274:MET:CE	2.86	0.53
1:I:187:GLU:HG3	1:I:229:LYS:O	2.08	0.53
1:L:14:GLU:OE2	1:L:138:LYS:NZ	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:93:PHE:O	1:Q:94:ARG:C	2.46	0.53
1:A:229:LYS:HG3	1:A:268:CYS:O	2.09	0.53
1:G:156:GLN:HB3	1:H:1:ALA:CA	2.39	0.53
1:N:313:TRP:CD2	1:N:315:GLY:CA	2.92	0.53
1:O:3:ARG:O	1:O:4:PHE:C	2.47	0.53
1:Q:148:ARG:HD2	3:Q:2008:HOH:O	2.09	0.53
1:F:12:LYS:HE2	1:F:222:TYR:CD1	2.44	0.52
1:K:212:VAL:O	1:K:215:ALA:HB3	2.09	0.52
1:L:62:LEU:O	1:L:65:VAL:HG13	2.09	0.52
1:M:198:LEU:CD1	1:M:234:THR:HA	2.39	0.52
1:P:150:VAL:HG13	1:P:191:ILE:HG13	1.91	0.52
1:D:80:HIS:CD2	1:D:137:TYR:OH	2.62	0.52
1:D:271:SER:HB3	1:D:301:TYR:CD2	2.44	0.52
1:E:282:ASN:O	1:E:286:ILE:HG13	2.10	0.52
1:F:319:ASN:O	1:F:320:LYS:C	2.47	0.52
1:J:119:ASN:O	1:J:152:ARG:NH1	2.39	0.52
1:L:97:LEU:O	1:L:98:LYS:C	2.45	0.52
1:M:352:SER:HA	1:M:354:GLN:CB	2.40	0.52
1:M:156:GLN:OE1	1:N:2:HIS:HB3	2.09	0.52
1:O:271:SER:O	1:O:272:GLY:C	2.48	0.52
1:R:254:THR:O	1:R:258:ARG:HG2	2.09	0.52
1:B:22:ILE:CG2	1:B:22:ILE:O	2.57	0.52
1:H:226:THR:HG21	3:H:421:HOH:O	2.06	0.52
1:I:119:ASN:HB2	1:J:4:PHE:CZ	2.44	0.52
1:J:330:ARG:NH1	1:J:347:SER:N	2.54	0.52
1:K:313:TRP:CE2	1:K:315:GLY:HA2	2.44	0.52
1:P:190:VAL:H	1:P:231:ASN:ND2	2.07	0.52
1:Q:275:SER:OG	1:Q:278:ASP:HB2	2.09	0.52
1:B:204:VAL:O	1:B:208:VAL:HG23	2.10	0.52
1:B:198:LEU:HD21	1:B:251:ALA:HB2	1.90	0.52
1:B:50:ASN:HD21	1:B:55:ARG:HH11	1.56	0.52
1:G:313:TRP:CH2	1:G:315:GLY:HA2	2.45	0.52
1:H:224:GLU:OE1	1:H:224:GLU:N	2.34	0.52
1:I:119:ASN:N	1:J:1:ALA:H3	2.07	0.52
1:M:44:GLN:OE1	1:M:44:GLN:HA	2.09	0.52
1:N:44:GLN:CA	1:N:44:GLN:OE1	2.56	0.52
1:D:121:GLU:OE1	1:D:159:SER:HB3	2.09	0.52
1:E:118:THR:CG2	1:E:121:GLU:H	2.21	0.52
1:F:276:GLU:HG3	1:F:352:SER:CB	2.40	0.52
1:H:191:ILE:CD1	1:H:191:ILE:N	2.71	0.52
1:K:191:ILE:HD13	1:K:192:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:SER:OG	1:K:348:SER:HA	2.08	0.52
1:L:65:VAL:O	1:L:100:LYS:NZ	2.33	0.52
1:Q:233:VAL:CG2	1:Q:252:THR:HA	2.40	0.52
1:A:147:TRP:HB2	1:A:173:TYR:CZ	2.45	0.52
1:A:199:GLU:HB2	3:A:566:HOH:O	2.08	0.52
1:G:80:HIS:HD2	1:G:137:TYR:OH	1.92	0.52
1:H:354:GLN:CG	1:H:356:LEU:HD23	2.39	0.52
1:I:12:LYS:HG2	1:I:222:TYR:CE2	2.44	0.52
1:N:42:ARG:CZ	1:N:303:ARG:HD3	2.40	0.52
1:O:106:ILE:HG22	1:O:142:VAL:HG11	1.91	0.52
1:O:155:ASP:O	1:O:156:GLN:HB2	2.10	0.52
1:A:91:LYS:HD3	1:A:96:ILE:CG1	2.40	0.52
1:B:87:ASP:O	1:B:88:SER:CB	2.58	0.52
1:C:54:ASN:O	1:C:55:ARG:C	2.48	0.52
1:F:231:ASN:ND2	1:F:231:ASN:H	2.06	0.52
1:F:91:LYS:NZ	1:F:99:GLU:OE1	2.42	0.52
1:N:80:HIS:CD2	1:N:137:TYR:OH	2.59	0.52
1:O:172:ARG:HD2	3:O:510:HOH:O	2.09	0.52
1:R:33:ASP:O	1:R:107:LYS:HE2	2.10	0.52
1:B:179:GLN:HG2	3:B:403:HOH:O	2.09	0.52
1:B:207:LYS:NZ	1:C:2:HIS:NE2	2.58	0.52
1:G:275:SER:OG	1:G:278:ASP:HB2	2.10	0.52
1:K:190:VAL:H	1:K:231:ASN:ND2	2.08	0.52
1:L:27:LYS:HG2	1:L:72:SER:O	2.10	0.52
1:L:337:ALA:O	1:L:338:ALA:C	2.42	0.52
1:N:231:ASN:ND2	1:N:231:ASN:H	2.07	0.52
1:N:250:MET:CE	1:N:291:LEU:HD21	2.40	0.52
1:N:52:GLU:HB2	1:N:55:ARG:NH2	2.25	0.52
1:O:76:VAL:HG23	1:O:102:ILE:HG21	1.92	0.52
1:O:3:ARG:CG	1:O:4:PHE:H	2.12	0.52
1:P:150:VAL:CG1	1:P:191:ILE:HG13	2.39	0.52
1:P:45:ARG:NH1	1:P:356:LEU:HA	2.24	0.52
1:P:3:ARG:CD	1:P:4:PHE:N	2.66	0.52
1:R:58:PHE:CE2	1:R:310:LEU:HD13	2.44	0.52
1:R:70:ASN:ND2	1:R:100:LYS:O	2.41	0.52
1:B:291:LEU:HB3	1:B:292:PRO:CD	2.40	0.52
1:C:30:LEU:HD12	1:C:31:ALA:N	2.24	0.52
1:F:250:MET:HE3	1:F:291:LEU:HD21	1.90	0.52
1:H:271:SER:HA	1:H:274:MET:CE	2.40	0.52
1:L:78:LEU:N	1:L:105:GLY:O	2.33	0.52
1:N:105:GLY:HA2	1:N:142:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:313:TRP:CD2	1:N:315:GLY:N	2.77	0.52
1:P:276:GLU:H	1:P:352:SER:CB	2.23	0.52
1:Q:112:GLY:HA2	1:Q:123:THR:O	2.09	0.52
1:A:187:GLU:O	1:A:187:GLU:HG2	2.09	0.52
1:F:187:GLU:HG2	1:F:187:GLU:O	2.10	0.52
1:H:67:SER:O	1:H:70:ASN:HB2	2.10	0.52
1:I:229:LYS:NZ	1:I:300:SER:OG	2.36	0.52
1:I:118:THR:CB	1:J:1:ALA:N	2.73	0.52
1:I:263:ALA:HA	1:L:257:HIS:CD2	2.44	0.52
1:O:118:THR:HG23	1:O:121:GLU:HB2	1.91	0.52
1:A:8:THR:OG1	1:A:11:GLN:HG3	2.10	0.51
1:A:128:ASP:N	1:B:128:ASP:OD2	2.41	0.51
1:G:119:ASN:N	1:H:1:ALA:N	2.48	0.51
1:H:281:LEU:CD2	1:H:344:HIS:CE1	2.93	0.51
1:H:350:ALA:O	1:H:354:GLN:HB2	2.09	0.51
1:O:276:GLU:HB3	3:O:504:HOH:O	2.10	0.51
1:Q:231:ASN:HA	1:Q:270:LEU:HG	1.92	0.51
1:C:232:MET:HG2	1:C:286:ILE:HD11	1.91	0.51
1:I:51:THR:HG21	1:I:53:GLU:HB3	1.92	0.51
1:I:51:THR:CG2	1:I:53:GLU:N	2.62	0.51
1:I:63:PHE:HB3	1:I:97:LEU:HD21	1.92	0.51
1:J:279:ALA:HB1	1:J:301:TYR:CE1	2.45	0.51
1:O:244:THR:HG23	1:O:246:GLU:OE1	2.10	0.51
1:P:298:SER:OG	1:P:299:PHE:N	2.43	0.51
1:A:45:ARG:HH12	1:A:356:LEU:HA	1.75	0.51
1:A:45:ARG:NH2	1:A:358:THR:N	2.51	0.51
1:B:198:LEU:CD1	1:B:234:THR:HA	2.40	0.51
1:E:244:THR:CG2	1:E:247:GLN:HG3	2.40	0.51
1:E:303:ARG:CG	1:E:303:ARG:NH1	2.73	0.51
1:F:226:THR:CG2	3:F:449:HOH:O	2.51	0.51
1:I:189:GLU:HG3	1:I:270:LEU:CD2	2.40	0.51
1:K:123:THR:CG2	1:K:124:ILE:H	2.13	0.51
1:Q:313:TRP:CH2	1:Q:315:GLY:HA2	2.44	0.51
1:B:79:PHE:O	1:B:80:HIS:C	2.49	0.51
1:B:207:LYS:NZ	1:C:2:HIS:CD2	2.78	0.51
1:A:203:TYR:CE2	1:D:2:HIS:HD2	2.16	0.51
1:G:156:GLN:HB3	1:H:1:ALA:CB	2.41	0.51
1:H:276:GLU:CB	1:H:352:SER:HB3	2.40	0.51
1:I:130:LEU:O	1:I:131:SER:C	2.48	0.51
1:K:244:THR:HG23	1:K:246:GLU:H	1.76	0.51
1:N:197:ASP:C	1:N:197:ASP:OD1	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:231:ASN:ND2	1:O:231:ASN:H	2.08	0.51
1:O:81:GLU:HG2	1:O:82:THR:N	2.25	0.51
1:Q:276:GLU:OE1	1:Q:308:SER:OG	2.19	0.51
1:R:173:TYR:CE1	1:R:177:CYS:SG	3.03	0.51
1:A:303:ARG:CB	1:A:357:PHE:HD1	2.24	0.51
1:B:244:THR:CG2	1:B:244:THR:O	2.59	0.51
1:B:56:ARG:HD2	1:B:86:LYS:O	2.11	0.51
1:C:237:HIS:ND1	3:C:403:HOH:O	2.34	0.51
1:D:319:ASN:O	1:D:320:LYS:C	2.49	0.51
1:E:148:ARG:NH1	1:E:189:GLU:OE1	2.42	0.51
1:F:138:LYS:NZ	1:F:181:GLY:O	2.39	0.51
1:G:200:HIS:HB2	3:G:563:HOH:O	2.10	0.51
1:I:125:GLN:HE22	1:J:129:GLY:H	1.57	0.51
1:K:119:ASN:O	1:K:152:ARG:NH1	2.43	0.51
1:Q:123:THR:HG21	1:Q:165:GLU:OE2	2.11	0.51
1:Q:187:GLU:HG2	1:Q:187:GLU:O	2.10	0.51
1:C:298:SER:OG	1:C:299:PHE:N	2.44	0.51
1:D:190:VAL:H	1:D:231:ASN:HD22	1.58	0.51
1:K:357:PHE:O	1:O:139:LYS:CE	2.55	0.51
1:L:61:ILE:HG22	1:L:324:GLN:HG2	1.93	0.51
1:M:68:SER:C	1:M:70:ASN:H	2.13	0.51
1:O:244:THR:HG22	1:O:247:GLN:HG3	1.91	0.51
1:P:38:THR:HG23	1:P:358:THR:HG21	1.92	0.51
1:Q:161:LEU:O	1:Q:165:GLU:HB3	2.11	0.51
1:A:147:TRP:HB2	1:A:173:TYR:CE1	2.45	0.51
1:A:343:VAL:HG12	1:A:343:VAL:O	2.08	0.51
1:C:80:HIS:HD2	1:C:137:TYR:OH	1.94	0.51
1:E:303:ARG:HG3	1:E:303:ARG:NH1	2.23	0.51
1:H:121:GLU:OE2	1:H:158:PRO:HA	2.09	0.51
1:H:45:ARG:HH12	1:H:356:LEU:HA	1.74	0.51
1:H:51:THR:O	1:H:52:GLU:C	2.48	0.51
1:I:51:THR:HG22	1:I:54:ASN:N	2.25	0.51
1:Q:217:ASN:ND2	3:Q:2002:HOH:O	2.43	0.51
1:E:1:ALA:HA	1:E:220:HIS:CE1	2.46	0.51
1:F:108:LEU:HD22	1:F:130:LEU:HD11	1.92	0.51
1:H:284:ASN:HB2	1:H:337:ALA:HB1	1.92	0.51
1:H:354:GLN:CG	1:H:356:LEU:CD2	2.88	0.51
1:I:105:GLY:HA2	1:I:142:VAL:HG13	1.93	0.51
1:I:313:TRP:CE2	1:I:315:GLY:CA	2.91	0.51
1:I:53:GLU:O	1:I:57:GLN:HB2	2.11	0.51
1:L:94:ARG:NH1	1:L:140:ASP:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:THR:CG2	1:M:121:GLU:N	2.63	0.51
1:R:244:THR:HG23	1:R:246:GLU:N	2.26	0.51
1:A:45:ARG:NH2	1:A:357:PHE:HA	2.20	0.51
1:C:124:ILE:CG2	1:C:147:TRP:CZ2	2.94	0.51
1:C:313:TRP:CD2	1:C:315:GLY:HA2	2.45	0.51
1:D:80:HIS:HD2	1:D:137:TYR:OH	1.94	0.51
1:E:2:HIS:O	1:E:4:PHE:CD1	2.63	0.51
1:G:146:LYS:HG2	1:G:147:TRP:N	2.26	0.51
1:I:244:THR:O	1:I:244:THR:CG2	2.59	0.51
1:I:244:THR:O	1:I:247:GLN:N	2.41	0.51
1:I:3:ARG:O	1:I:4:PHE:C	2.48	0.51
1:K:119:ASN:OD1	1:K:119:ASN:C	2.48	0.51
1:K:50:ASN:HD21	1:K:55:ARG:HH11	1.56	0.51
1:M:345:THR:HB	1:M:347:SER:OG	2.11	0.51
1:O:179:GLN:HG2	3:O:502:HOH:O	2.11	0.51
1:E:28:GLY:HA3	1:E:299:PHE:CE1	2.46	0.51
1:F:256:LEU:CD1	1:F:267:ILE:CD1	2.89	0.51
1:F:306:GLN:HA	3:F:414:HOH:O	2.11	0.51
1:G:18:ILE:CD1	1:G:143:ASP:HB3	2.35	0.51
1:G:271:SER:HA	1:G:274:MET:HE3	1.92	0.51
1:H:284:ASN:HB2	1:H:337:ALA:CB	2.41	0.51
1:I:244:THR:CG2	1:I:247:GLN:N	2.74	0.51
1:I:2:HIS:HB3	1:J:156:GLN:CD	2.30	0.51
1:J:65:VAL:O	1:J:100:LYS:NZ	2.38	0.51
1:L:146:LYS:HB2	1:L:185:ILE:HB	1.93	0.51
1:N:189:GLU:CG	1:N:191:ILE:HD12	2.40	0.51
1:N:83:LEU:HD23	1:N:84:TYR:CZ	2.45	0.51
1:P:244:THR:HG23	1:P:246:GLU:N	2.26	0.51
1:R:202:GLN:HB2	1:R:233:VAL:HG11	1.92	0.51
1:E:319:ASN:O	1:E:320:LYS:C	2.48	0.50
1:F:124:ILE:HD13	1:F:149:ALA:HA	1.93	0.50
1:I:272:GLY:HA2	1:I:303:ARG:HH12	1.76	0.50
1:L:190:VAL:HB	1:L:231:ASN:ND2	2.26	0.50
1:L:52:GLU:HA	1:L:55:ARG:NH2	2.26	0.50
1:O:65:VAL:CG2	1:O:328:MET:HE2	2.40	0.50
1:A:244:THR:O	1:A:247:GLN:N	2.44	0.50
1:B:56:ARG:HB2	1:B:85:GLN:NE2	2.26	0.50
1:D:250:MET:HE3	1:D:291:LEU:CD2	2.40	0.50
1:E:25:ASN:H	1:E:27:LYS:HG3	1.76	0.50
1:E:25:ASN:H	1:E:27:LYS:H	1.58	0.50
1:H:189:GLU:HG2	1:H:191:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:LYS:HA	1:H:268:CYS:O	2.10	0.50
1:J:94:ARG:HD3	1:J:140:ASP:O	2.11	0.50
1:L:256:LEU:HD22	1:L:267:ILE:CD1	2.42	0.50
1:L:256:LEU:HD22	1:L:267:ILE:HD12	1.92	0.50
1:L:283:LEU:HD11	1:L:297:LEU:O	2.11	0.50
1:O:1:ALA:O	1:O:2:HIS:HB2	2.11	0.50
1:O:215:ALA:O	1:O:218:ASP:HB2	2.11	0.50
1:O:336:GLN:HA	1:O:339:LYS:HD2	1.93	0.50
1:Q:126:GLY:H	1:R:128:ASP:CG	2.14	0.50
1:R:343:VAL:O	1:R:344:HIS:CB	2.58	0.50
1:B:276:GLU:OE2	1:B:307:ALA:HB3	2.11	0.50
1:B:65:VAL:HG13	1:B:66:ASP:N	2.25	0.50
1:D:119:ASN:O	1:D:120:LYS:HB2	2.10	0.50
1:D:155:ASP:O	1:D:156:GLN:HB2	2.10	0.50
1:D:233:VAL:N	1:D:252:THR:OG1	2.32	0.50
1:D:86:LYS:HB3	1:D:90:GLY:HA2	1.93	0.50
1:F:109:ASP:HA	1:F:147:TRP:CE3	2.47	0.50
1:F:213:TYR:OH	1:F:228:LEU:HD13	2.11	0.50
1:H:8:THR:HB	1:H:11:GLN:HG3	1.93	0.50
1:I:128:ASP:OD2	1:J:128:ASP:N	2.39	0.50
1:I:76:VAL:HG23	1:I:102:ILE:HG21	1.92	0.50
1:L:245:PRO:O	1:L:249:ALA:N	2.40	0.50
1:N:51:THR:HG22	1:N:53:GLU:N	2.27	0.50
1:R:344:HIS:CD2	3:R:566:HOH:O	2.64	0.50
1:D:87:ASP:CB	1:D:89:GLN:O	2.59	0.50
1:H:276:GLU:HB2	1:H:352:SER:HB3	1.93	0.50
1:H:58:PHE:CE2	1:H:310:LEU:HD13	2.46	0.50
1:H:313:TRP:CE2	1:H:315:GLY:HA2	2.47	0.50
1:I:36:VAL:HG13	1:I:55:ARG:CZ	2.42	0.50
1:J:271:SER:HB3	1:J:301:TYR:CD2	2.46	0.50
1:M:1:ALA:H2	1:N:118:THR:CB	2.23	0.50
1:P:276:GLU:HG3	1:P:352:SER:CB	2.40	0.50
1:R:51:THR:CG2	1:R:54:ASN:H	1.99	0.50
1:C:118:THR:HG22	1:C:121:GLU:H	1.70	0.50
1:A:207:LYS:CE	1:D:2:HIS:HE2	2.24	0.50
1:D:276:GLU:OE2	1:D:307:ALA:HB3	2.11	0.50
1:H:158:PRO:O	1:H:158:PRO:HG2	2.12	0.50
1:I:46:ILE:HG13	1:I:48:VAL:HG23	1.94	0.50
1:J:313:TRP:CZ2	1:J:315:GLY:HA2	2.47	0.50
1:K:357:PHE:C	1:O:139:LYS:CE	2.80	0.50
1:L:118:THR:CG2	1:L:121:GLU:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:GLN:NE2	1:L:3:ARG:NE	2.59	0.50
1:M:80:HIS:CD2	1:M:137:TYR:OH	2.64	0.50
1:R:44:GLN:OE1	1:R:44:GLN:HA	2.12	0.50
1:A:154:ALA:O	1:A:155:ASP:C	2.47	0.50
1:A:66:ASP:OD1	1:A:66:ASP:C	2.50	0.50
1:C:185:ILE:HG22	1:C:185:ILE:O	2.11	0.50
1:C:282:ASN:O	1:C:286:ILE:HG13	2.11	0.50
1:I:128:ASP:OD1	1:J:126:GLY:N	2.41	0.50
1:I:274:MET:CE	1:I:279:ALA:HA	2.42	0.50
1:M:3:ARG:NH1	1:N:156:GLN:HE21	2.06	0.50
1:O:196:HIS:O	1:O:239:CYS:HB2	2.11	0.50
1:P:115:LEU:HD22	1:P:122:THR:C	2.32	0.50
1:Q:80:HIS:HD2	1:Q:137:TYR:OH	1.94	0.50
1:Q:147:TRP:HB3	1:Q:173:TYR:CE2	2.46	0.50
1:A:313:TRP:CD2	1:A:315:GLY:HA2	2.46	0.50
1:D:2:HIS:O	1:D:4:PHE:CD1	2.61	0.50
1:J:121:GLU:OE2	1:J:158:PRO:HA	2.12	0.50
1:O:220:HIS:CE1	3:O:528:HOH:O	2.56	0.50
1:O:244:THR:HB	1:O:247:GLN:OE1	2.11	0.50
1:A:121:GLU:OE2	1:A:158:PRO:HA	2.12	0.50
1:A:303:ARG:HB3	1:A:356:LEU:HD13	1.94	0.50
1:D:105:GLY:HA2	1:D:144:PHE:O	2.12	0.50
1:D:60:GLU:HB2	1:D:93:PHE:CE1	2.47	0.50
1:E:190:VAL:HB	1:E:231:ASN:ND2	2.26	0.50
1:E:271:SER:HA	1:E:274:MET:HE1	1.93	0.50
1:I:75:GLY:HA2	1:I:103:VAL:O	2.12	0.50
1:L:271:SER:O	1:L:272:GLY:C	2.48	0.50
1:N:299:PHE:CD1	1:N:299:PHE:N	2.78	0.50
1:M:46:ILE:O	1:M:47:LYS:C	2.50	0.50
1:N:61:ILE:HG22	1:N:324:GLN:HG2	1.92	0.50
1:A:222:TYR:CZ	1:A:224:GLU:HB2	2.47	0.49
1:B:343:VAL:O	1:B:345:THR:N	2.45	0.49
1:F:123:THR:CG2	1:F:165:GLU:CG	2.90	0.49
1:G:249:ALA:HB1	1:G:286:ILE:HA	1.93	0.49
1:G:3:ARG:HD2	3:G:574:HOH:O	2.12	0.49
1:J:161:LEU:O	1:J:165:GLU:HB3	2.12	0.49
1:J:349:GLY:O	1:J:350:ALA:C	2.51	0.49
1:K:123:THR:HG23	1:K:165:GLU:HG3	1.93	0.49
1:M:65:VAL:CG1	1:M:328:MET:SD	3.00	0.49
1:P:303:ARG:NE	1:P:356:LEU:O	2.41	0.49
1:R:172:ARG:O	1:R:176:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HB3	1:A:357:PHE:HD1	1.77	0.49
1:A:2:HIS:CB	1:A:3:ARG:HD2	2.22	0.49
1:B:244:THR:O	1:B:245:PRO:C	2.50	0.49
1:C:244:THR:CG2	1:C:247:GLN:N	2.74	0.49
1:C:277:GLU:O	1:C:281:LEU:HG	2.11	0.49
1:I:226:THR:CG2	3:I:423:HOH:O	2.48	0.49
1:M:123:THR:HG22	1:M:124:ILE:N	2.19	0.49
1:M:271:SER:HA	1:M:274:MET:HE3	1.95	0.49
1:N:244:THR:N	1:N:247:GLN:OE1	2.45	0.49
1:O:75:GLY:HA2	1:O:103:VAL:O	2.12	0.49
1:O:198:LEU:CD1	1:O:234:THR:HA	2.43	0.49
1:O:58:PHE:CE1	1:O:310:LEU:CD1	2.92	0.49
1:O:80:HIS:HD2	1:O:137:TYR:OH	1.95	0.49
1:R:214:LYS:HE3	1:R:218:ASP:OD1	2.12	0.49
1:C:1:ALA:HB1	1:C:4:PHE:HD1	1.77	0.49
1:D:51:THR:O	1:D:52:GLU:C	2.49	0.49
1:E:123:THR:CG2	1:E:165:GLU:HG3	2.42	0.49
1:E:313:TRP:CZ2	1:E:315:GLY:HA2	2.47	0.49
1:F:123:THR:HG23	1:F:165:GLU:HG3	1.95	0.49
1:G:3:ARG:HE	1:H:156:GLN:HE21	1.59	0.49
1:G:3:ARG:HG2	1:G:3:ARG:NH1	2.23	0.49
1:H:106:ILE:HG23	1:H:106:ILE:O	2.11	0.49
1:N:250:MET:HE3	1:N:291:LEU:HD21	1.93	0.49
1:R:10:GLU:OE1	3:R:501:HOH:O	2.17	0.49
1:A:33:ASP:O	1:A:107:LYS:HE3	2.12	0.49
1:A:66:ASP:OD1	1:A:67:SER:HB2	2.12	0.49
1:B:333:ALA:O	1:B:336:GLN:HB2	2.13	0.49
1:C:232:MET:HG2	1:C:286:ILE:CD1	2.42	0.49
1:D:329:LYS:HE2	1:D:347:SER:N	2.27	0.49
1:H:220:HIS:CE1	3:H:407:HOH:O	2.62	0.49
1:H:351:ALA:O	1:H:352:SER:HB2	2.12	0.49
1:H:349:GLY:HA2	1:H:353:THR:HG23	1.94	0.49
1:I:258:ARG:HH11	1:L:224:GLU:CD	2.15	0.49
1:J:231:ASN:H	1:J:231:ASN:ND2	2.11	0.49
1:J:329:LYS:HE2	1:J:346:GLY:O	2.11	0.49
1:L:155:ASP:OD1	1:L:156:GLN:HG3	2.12	0.49
1:M:342:TYR:OH	1:M:345:THR:OG1	2.28	0.49
1:P:115:LEU:O	1:P:118:THR:HB	2.13	0.49
1:Q:9:GLN:HG2	3:Q:2031:HOH:O	2.12	0.49
1:R:123:THR:HG23	1:R:165:GLU:HG3	1.94	0.49
1:B:66:ASP:O	1:B:68:SER:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:ASP:OD1	1:H:66:ASP:O	2.30	0.49
1:I:44:GLN:CA	1:I:44:GLN:OE1	2.58	0.49
1:I:156:GLN:NE2	1:J:4:PHE:HE1	2.10	0.49
1:J:66:ASP:OD1	1:J:68:SER:HB2	2.13	0.49
1:K:276:GLU:HB3	1:K:330:ARG:HH11	1.78	0.49
1:L:282:ASN:O	1:L:286:ILE:HG13	2.12	0.49
1:N:3:ARG:NH1	1:O:203:TYR:CE2	2.80	0.49
1:O:94:ARG:O	1:O:98:LYS:HB2	2.12	0.49
1:B:244:THR:HG23	1:B:247:GLN:H	1.70	0.49
1:B:69:ILE:O	1:B:71:GLN:N	2.46	0.49
1:C:80:HIS:CD2	1:C:137:TYR:OH	2.65	0.49
1:C:229:LYS:HG3	1:C:268:CYS:O	2.13	0.49
1:C:275:SER:O	1:C:276:GLU:C	2.48	0.49
1:H:276:GLU:OE1	1:H:330:ARG:HD3	2.12	0.49
1:K:33:ASP:OD1	1:K:33:ASP:N	2.45	0.49
1:L:51:THR:CG2	1:L:54:ASN:N	2.59	0.49
1:M:349:GLY:C	1:M:351:ALA:H	2.15	0.49
1:N:8:THR:O	1:N:9:GLN:C	2.50	0.49
1:P:51:THR:HG22	1:P:54:ASN:CB	2.43	0.49
1:A:51:THR:HG22	1:A:53:GLU:N	2.28	0.49
1:J:29:ILE:HB	1:J:300:SER:HA	1.94	0.49
1:K:229:LYS:HA	1:K:268:CYS:O	2.11	0.49
1:K:65:VAL:HG12	1:K:324:GLN:HB3	1.94	0.49
1:K:119:ASN:HB2	1:L:4:PHE:CE1	2.48	0.49
1:N:25:ASN:H	1:N:27:LYS:HG3	1.78	0.49
1:N:91:LYS:NZ	1:N:99:GLU:OE1	2.45	0.49
1:O:343:VAL:O	1:O:344:HIS:CG	2.66	0.49
1:Q:271:SER:O	1:Q:272:GLY:C	2.50	0.49
1:R:257:HIS:HD2	1:R:292:PRO:HD2	1.73	0.49
1:A:8:THR:N	1:A:11:GLN:OE1	2.37	0.49
1:D:293:LYS:HA	1:D:295:TRP:CZ3	2.47	0.49
1:G:226:THR:CG2	3:G:506:HOH:O	2.61	0.49
1:G:3:ARG:CG	1:G:3:ARG:NH1	2.73	0.49
1:J:112:GLY:HA2	1:J:123:THR:O	2.13	0.49
1:J:67:SER:O	1:J:68:SER:C	2.51	0.49
1:K:344:HIS:ND1	1:K:346:GLY:N	2.61	0.49
1:L:48:VAL:HG12	1:L:54:ASN:ND2	2.26	0.49
1:B:252:THR:HG22	1:B:253:VAL:N	2.25	0.49
1:C:29:ILE:HB	1:C:300:SER:HA	1.93	0.49
1:D:66:ASP:OD2	1:D:68:SER:HB2	2.13	0.49
1:E:80:HIS:HD2	1:E:137:TYR:OH	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ASP:C	1:E:89:GLN:HB3	2.33	0.49
1:G:250:MET:HG2	1:G:289:CYS:SG	2.53	0.49
1:I:313:TRP:CH2	1:I:315:GLY:HA2	2.48	0.49
1:I:38:THR:O	1:I:41:ASN:N	2.46	0.49
1:J:329:LYS:CD	1:J:347:SER:HA	2.36	0.49
1:M:329:LYS:HE3	1:M:348:SER:H	1.78	0.49
1:M:329:LYS:NZ	1:M:348:SER:N	2.57	0.49
1:O:335:CYS:SG	1:O:339:LYS:HE2	2.53	0.49
1:P:123:THR:HG22	1:P:124:ILE:N	2.23	0.49
1:Q:50:ASN:ND2	1:Q:55:ARG:HD3	2.20	0.49
1:R:62:LEU:O	1:R:65:VAL:HG13	2.13	0.49
1:C:295:TRP:O	1:C:296:LYS:C	2.50	0.49
1:C:42:ARG:O	1:C:45:ARG:HB2	2.13	0.49
1:D:354:GLN:HG2	1:D:356:LEU:HD21	1.95	0.49
1:F:118:THR:HG21	1:F:121:GLU:HB2	1.91	0.49
1:G:33:ASP:CB	1:G:77:ILE:HG22	2.42	0.49
1:G:46:ILE:O	1:G:47:LYS:C	2.51	0.49
1:G:65:VAL:O	1:G:66:ASP:CB	2.59	0.49
1:J:199:GLU:CB	3:J:534:HOH:O	2.61	0.49
1:K:133:ARG:HH11	1:K:133:ARG:HD3	1.02	0.49
1:K:357:PHE:C	1:K:357:PHE:CD1	2.83	0.49
1:L:294:PRO:HD2	1:L:295:TRP:CE2	2.48	0.49
1:M:86:LYS:HD3	1:M:90:GLY:HA2	1.95	0.49
1:N:113:ALA:HB2	1:N:125:GLN:HE21	1.78	0.49
1:N:319:ASN:O	1:N:320:LYS:C	2.50	0.49
1:Q:244:THR:HG22	1:Q:247:GLN:CB	2.43	0.49
1:A:8:THR:HG23	1:A:11:GLN:OE1	2.13	0.48
1:C:244:THR:HG21	1:C:247:GLN:HG3	1.93	0.48
1:E:23:VAL:HG23	1:E:296:LYS:HG3	1.94	0.48
1:F:95:ASN:O	1:F:99:GLU:HG3	2.13	0.48
1:G:322:ALA:O	1:G:325:GLU:HB2	2.12	0.48
1:J:80:HIS:HD2	1:J:137:TYR:OH	1.95	0.48
1:N:244:THR:HG22	1:N:247:GLN:CB	2.42	0.48
1:N:254:THR:O	1:N:258:ARG:HG2	2.13	0.48
1:O:4:PHE:CE1	1:P:119:ASN:HB2	2.48	0.48
1:P:254:THR:O	1:P:258:ARG:HG2	2.13	0.48
1:Q:256:LEU:CD1	1:Q:267:ILE:HD11	2.43	0.48
1:R:131:SER:HB2	3:R:554:HOH:O	2.12	0.48
1:R:60:GLU:OE1	1:R:87:ASP:HB2	2.12	0.48
1:A:125:GLN:HE22	1:B:129:GLY:N	1.96	0.48
1:A:12:LYS:HG2	1:A:222:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:CD	1:B:156:GLN:HE22	2.27	0.48
1:B:97:LEU:O	1:B:98:LYS:C	2.51	0.48
1:C:123:THR:CG2	1:C:124:ILE:N	2.72	0.48
1:D:146:LYS:HE2	1:D:187:GLU:OE1	2.12	0.48
1:D:244:THR:CG2	1:D:246:GLU:HB2	2.44	0.48
1:D:343:VAL:CG1	1:D:344:HIS:N	2.76	0.48
1:E:274:MET:HB2	1:E:274:MET:HE2	1.52	0.48
1:F:256:LEU:HD13	1:F:267:ILE:HD13	1.96	0.48
1:F:276:GLU:HB2	1:F:352:SER:HB3	1.95	0.48
1:H:231:ASN:ND2	1:H:231:ASN:H	2.11	0.48
1:J:124:ILE:HG22	1:J:147:TRP:CZ2	2.48	0.48
1:K:118:THR:HG23	1:K:121:GLU:H	1.77	0.48
1:K:144:PHE:HB2	1:K:183:VAL:O	2.12	0.48
1:K:28:GLY:HA3	1:K:299:PHE:CZ	2.48	0.48
1:L:313:TRP:HB2	1:L:323:THR:OG1	2.13	0.48
1:A:66:ASP:OD1	1:A:67:SER:N	2.45	0.48
1:B:313:TRP:HB2	1:B:323:THR:OG1	2.13	0.48
1:B:66:ASP:C	1:B:66:ASP:OD1	2.52	0.48
1:E:244:THR:HG23	1:E:246:GLU:OE1	2.12	0.48
1:G:164:GLN:O	1:G:168:ASN:ND2	2.47	0.48
1:K:268:CYS:HB3	1:K:300:SER:HB2	1.96	0.48
1:M:329:LYS:HE3	1:M:348:SER:N	2.28	0.48
1:O:128:ASP:OD1	1:P:125:GLN:HB3	2.12	0.48
1:O:278:ASP:O	1:O:280:THR:N	2.47	0.48
1:O:66:ASP:O	1:O:67:SER:C	2.50	0.48
1:Q:123:THR:HG23	1:Q:165:GLU:HG3	1.94	0.48
1:R:127:LEU:O	1:R:128:ASP:C	2.51	0.48
1:B:118:THR:CG2	1:B:121:GLU:N	2.68	0.48
1:D:226:THR:CG2	3:D:541:HOH:O	2.48	0.48
1:H:277:GLU:CG	1:H:345:THR:HG23	2.37	0.48
1:I:68:SER:O	1:I:70:ASN:ND2	2.46	0.48
1:O:1:ALA:CB	1:P:159:SER:HB3	2.44	0.48
1:C:244:THR:HG23	1:C:246:GLU:H	1.77	0.48
1:F:25:ASN:H	1:F:27:LYS:H	1.61	0.48
1:F:352:SER:HA	1:F:354:GLN:HB3	1.96	0.48
1:F:65:VAL:HG22	1:F:328:MET:SD	2.54	0.48
1:G:187:GLU:HG3	1:G:229:LYS:CG	2.42	0.48
1:H:350:ALA:HA	1:H:353:THR:OG1	2.13	0.48
1:H:276:GLU:CG	1:H:352:SER:HB3	2.43	0.48
1:K:229:LYS:HG3	1:K:268:CYS:O	2.12	0.48
1:K:291:LEU:O	1:K:293:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:66:ASP:O	1:L:68:SER:N	2.47	0.48
1:O:187:GLU:HG3	1:O:229:LYS:HG2	1.95	0.48
1:Q:334:ASN:O	1:Q:338:ALA:N	2.41	0.48
1:A:3:ARG:HD3	1:B:156:GLN:HE22	1.75	0.48
1:B:3:ARG:O	1:B:4:PHE:C	2.51	0.48
1:C:64:SER:O	1:C:65:VAL:C	2.51	0.48
1:D:67:SER:O	1:D:70:ASN:N	2.44	0.48
1:E:352:SER:HA	1:E:354:GLN:H	1.79	0.48
1:G:32:ALA:HB1	3:G:510:HOH:O	2.13	0.48
1:H:354:GLN:HA	3:H:435:HOH:O	2.13	0.48
1:I:271:SER:HB3	1:I:301:TYR:CD2	2.48	0.48
1:L:58:PHE:CE2	1:L:62:LEU:HD21	2.49	0.48
1:M:123:THR:C	1:M:124:ILE:HD13	2.34	0.48
1:M:303:ARG:HD2	1:M:356:LEU:CB	2.43	0.48
1:N:218:ASP:HA	3:N:403:HOH:O	2.13	0.48
1:O:144:PHE:HB2	1:O:183:VAL:O	2.14	0.48
1:P:291:LEU:HB3	1:P:292:PRO:HD2	1.96	0.48
1:Q:92:LEU:O	1:Q:93:PHE:C	2.50	0.48
1:R:250:MET:O	1:R:250:MET:HG3	2.12	0.48
1:R:50:ASN:HD21	1:R:55:ARG:HD3	1.77	0.48
1:A:6:ALA:O	1:A:7:LEU:HD23	2.13	0.48
1:C:271:SER:CA	1:C:274:MET:HE2	2.43	0.48
1:C:87:ASP:OD2	1:C:91:LYS:HB3	2.13	0.48
1:F:51:THR:HG22	1:F:54:ASN:N	2.22	0.48
1:G:112:GLY:HA2	1:G:123:THR:O	2.13	0.48
1:I:36:VAL:HG13	1:I:55:ARG:NH1	2.29	0.48
1:L:3:ARG:O	1:L:4:PHE:C	2.51	0.48
1:M:123:THR:CG2	1:M:124:ILE:N	2.77	0.48
1:M:137:TYR:O	1:M:138:LYS:C	2.51	0.48
1:N:118:THR:HG23	1:N:121:GLU:HB2	1.96	0.48
1:N:58:PHE:CE1	1:N:310:LEU:HD12	2.49	0.48
1:O:58:PHE:CE2	1:O:62:LEU:HD11	2.49	0.48
1:Q:137:TYR:O	1:Q:138:LYS:C	2.50	0.48
1:Q:267:ILE:HD13	1:Q:267:ILE:HG21	1.57	0.48
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.49	0.48
1:A:58:PHE:CE1	1:A:310:LEU:HD13	2.49	0.48
2:A:402:SO4:O1	1:D:12:LYS:NZ	2.46	0.48
1:B:191:ILE:HA	1:B:191:ILE:HD13	1.41	0.48
1:D:28:GLY:O	1:D:74:GLY:N	2.38	0.48
1:D:329:LYS:NZ	1:D:347:SER:CA	2.72	0.48
1:E:244:THR:HG23	1:E:246:GLU:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:THR:O	1:F:242:LYS:HE3	2.14	0.48
1:G:67:SER:O	1:G:70:ASN:HB2	2.13	0.48
1:I:78:LEU:O	1:I:106:ILE:HD12	2.13	0.48
1:J:191:ILE:HD12	1:J:191:ILE:HG23	1.56	0.48
1:M:78:LEU:O	1:M:106:ILE:HD12	2.14	0.48
1:O:7:LEU:HB3	1:O:11:GLN:HB2	1.95	0.48
1:Q:33:ASP:OD2	1:Q:107:LYS:HE3	2.14	0.48
1:H:25:ASN:HB3	3:H:414:HOH:O	2.14	0.48
1:H:67:SER:HA	1:H:100:LYS:HD3	1.94	0.48
1:J:118:THR:HG22	1:J:121:GLU:H	1.75	0.48
1:J:124:ILE:HG21	1:J:147:TRP:NE1	2.29	0.48
1:K:91:LYS:HD3	1:K:96:ILE:CG1	2.44	0.48
1:M:352:SER:OG	1:M:354:GLN:HB3	2.13	0.48
1:N:78:LEU:O	1:N:106:ILE:HA	2.14	0.48
1:B:89:GLN:C	1:B:91:LYS:N	2.67	0.48
1:D:305:LEU:HD23	1:D:330:ARG:HB3	1.94	0.48
1:D:61:ILE:HG21	1:D:323:THR:HG21	1.95	0.48
1:I:204:VAL:O	1:I:207:LYS:N	2.45	0.48
1:J:93:PHE:N	3:J:506:HOH:O	2.46	0.48
1:K:128:ASP:HA	1:L:125:GLN:HE21	1.78	0.48
1:N:106:ILE:HG22	1:N:142:VAL:HG11	1.96	0.48
1:A:313:TRP:CZ2	1:A:315:GLY:HA2	2.48	0.47
1:F:38:THR:O	1:F:42:ARG:HG2	2.14	0.47
1:L:337:ALA:O	1:L:339:LYS:N	2.47	0.47
1:L:46:ILE:HD12	1:L:48:VAL:HG23	1.95	0.47
1:N:298:SER:OG	1:N:299:PHE:N	2.47	0.47
1:Q:18:ILE:HD13	1:Q:143:ASP:HB3	1.96	0.47
1:R:33:ASP:N	1:R:33:ASP:OD1	2.37	0.47
1:C:171:ALA:HA	1:C:216:LEU:HD12	1.96	0.47
1:D:187:GLU:HG3	1:D:229:LYS:HG2	1.97	0.47
1:E:76:VAL:HG23	1:E:102:ILE:HG21	1.96	0.47
1:F:123:THR:HG23	1:F:165:GLU:CG	2.44	0.47
1:H:309:ALA:O	1:H:323:THR:HG23	2.13	0.47
1:I:164:GLN:O	1:I:168:ASN:ND2	2.45	0.47
1:I:123:THR:HG21	1:I:165:GLU:OE2	2.14	0.47
1:J:319:ASN:O	1:J:320:LYS:C	2.53	0.47
1:K:171:ALA:HA	1:K:216:LEU:HD12	1.94	0.47
1:M:156:GLN:OE1	1:N:2:HIS:CA	2.62	0.47
1:R:280:THR:HG21	1:R:333:ALA:HB1	1.96	0.47
1:R:44:GLN:O	1:R:47:LYS:N	2.43	0.47
1:A:124:ILE:HD12	3:A:523:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:NZ	3:A:501:HOH:O	2.47	0.47
1:A:83:LEU:O	1:A:83:LEU:HG	2.14	0.47
1:B:29:ILE:O	1:B:300:SER:HA	2.14	0.47
1:G:250:MET:CE	1:G:291:LEU:CD2	2.93	0.47
1:I:189:GLU:HG3	1:I:270:LEU:HD21	1.96	0.47
1:L:276:GLU:OE2	1:L:307:ALA:HB3	2.14	0.47
1:P:118:THR:CG2	1:P:121:GLU:H	2.27	0.47
1:P:250:MET:HE1	1:P:291:LEU:HD11	1.95	0.47
1:Q:330:ARG:HA	1:Q:330:ARG:NE	2.29	0.47
1:A:244:THR:O	1:A:244:THR:HG22	2.14	0.47
1:C:2:HIS:O	1:C:3:ARG:HB2	2.15	0.47
1:E:87:ASP:O	1:E:89:GLN:HB2	2.14	0.47
1:G:121:GLU:OE2	1:G:158:PRO:HA	2.14	0.47
1:H:50:ASN:ND2	1:H:55:ARG:HH11	2.12	0.47
1:I:61:ILE:HG22	1:I:324:GLN:HG2	1.95	0.47
1:L:174:ALA:O	1:L:175:SER:C	2.53	0.47
1:N:33:ASP:HB3	1:N:77:ILE:HG22	1.95	0.47
1:N:284:ASN:ND2	1:N:342:TYR:H	2.11	0.47
1:O:226:THR:CG2	1:O:227:LEU:N	2.77	0.47
1:R:191:ILE:HB	1:R:192:PRO:CD	2.44	0.47
1:A:249:ALA:HB1	1:A:286:ILE:HA	1.95	0.47
1:B:18:ILE:O	1:B:22:ILE:HD12	2.14	0.47
1:E:260:VAL:HA	1:E:261:PRO:HD3	1.78	0.47
1:E:44:GLN:O	1:E:47:LYS:N	2.42	0.47
1:G:118:THR:CG2	1:G:121:GLU:HB2	2.43	0.47
1:G:219:HIS:O	1:G:220:HIS:CB	2.62	0.47
1:I:118:THR:C	1:J:1:ALA:H3	2.18	0.47
1:K:349:GLY:O	1:K:352:SER:HB2	2.14	0.47
1:L:59:ARG:HB3	1:L:63:PHE:CE1	2.49	0.47
1:M:221:VAL:CG1	1:M:222:TYR:N	2.77	0.47
1:N:294:PRO:HD2	1:N:295:TRP:CH2	2.49	0.47
1:O:230:PRO:CG	1:O:267:ILE:CD1	2.92	0.47
1:Q:80:HIS:CD2	1:Q:137:TYR:OH	2.68	0.47
1:R:244:THR:CG2	1:R:247:GLN:HG3	2.44	0.47
1:B:132:GLU:O	1:B:133:ARG:C	2.50	0.47
1:C:161:LEU:O	1:C:162:ALA:C	2.52	0.47
1:E:229:LYS:HA	1:E:268:CYS:O	2.14	0.47
1:E:245:PRO:HA	1:E:282:ASN:OD1	2.14	0.47
1:H:42:ARG:HD2	1:H:42:ARG:HH11	1.24	0.47
1:I:106:ILE:HG22	1:I:142:VAL:HG11	1.94	0.47
1:J:50:ASN:HD21	1:J:55:ARG:HH11	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:ILE:CA	1:M:71:GLN:N	2.61	0.47
1:Q:228:LEU:HG	1:Q:230:PRO:HD3	1.96	0.47
1:R:118:THR:CG2	1:R:121:GLU:H	2.27	0.47
1:R:124:ILE:CD1	3:R:514:HOH:O	2.59	0.47
1:A:50:ASN:HD21	1:A:55:ARG:HD3	1.79	0.47
1:B:67:SER:C	1:B:68:SER:O	2.52	0.47
1:C:105:GLY:HA3	1:C:144:PHE:CZ	2.49	0.47
1:C:51:THR:CG2	1:C:53:GLU:N	2.77	0.47
1:H:242:LYS:HA	1:H:242:LYS:HE2	1.96	0.47
1:H:2:HIS:O	1:H:3:ARG:CB	2.56	0.47
1:J:44:GLN:OE1	1:J:44:GLN:HA	2.14	0.47
1:K:79:PHE:O	1:K:80:HIS:C	2.52	0.47
1:M:144:PHE:HB2	1:M:183:VAL:O	2.14	0.47
1:M:158:PRO:HG3	1:M:204:VAL:HG13	1.97	0.47
1:P:8:THR:OG1	1:P:11:GLN:HG3	2.14	0.47
1:A:79:PHE:O	1:A:80:HIS:C	2.52	0.47
1:B:233:VAL:O	1:B:248:VAL:HG13	2.15	0.47
1:B:256:LEU:HD13	1:B:267:ILE:HD11	1.97	0.47
1:B:51:THR:HG23	1:B:54:ASN:H	1.69	0.47
1:B:58:PHE:CE2	1:B:62:LEU:HD11	2.49	0.47
1:D:147:TRP:HB3	1:D:173:TYR:CE2	2.49	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47
1:E:276:GLU:OE2	1:E:307:ALA:HB3	2.14	0.47
1:G:126:GLY:H	1:H:128:ASP:CG	2.18	0.47
1:G:298:SER:OG	1:G:299:PHE:N	2.48	0.47
1:H:105:GLY:HA3	1:H:144:PHE:CZ	2.50	0.47
1:J:120:LYS:HB2	1:J:152:ARG:HH12	1.80	0.47
1:J:330:ARG:NH1	1:J:346:GLY:CA	2.73	0.47
1:L:18:ILE:O	1:L:22:ILE:HG13	2.14	0.47
1:L:69:ILE:O	1:L:71:GLN:N	2.47	0.47
1:M:343:VAL:O	1:M:344:HIS:HB2	2.14	0.47
1:O:121:GLU:OE1	1:P:1:ALA:HB2	2.14	0.47
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.97	0.47
1:C:68:SER:O	1:C:71:GLN:HG3	2.15	0.47
1:D:29:ILE:HB	1:D:300:SER:HA	1.96	0.47
1:F:313:TRP:CZ2	1:F:315:GLY:HA2	2.50	0.47
1:F:329:LYS:CE	1:F:347:SER:CA	2.76	0.47
1:L:80:HIS:CD2	1:L:137:TYR:OH	2.68	0.47
1:M:303:ARG:HB3	1:M:356:LEU:HD13	1.97	0.47
1:N:50:ASN:HD21	1:N:55:ARG:HD3	1.80	0.47
1:N:9:GLN:CD	3:N:401:HOH:O	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:133:ARG:HH11	1:O:133:ARG:HD3	1.28	0.47
1:Q:244:THR:HG23	1:Q:247:GLN:H	1.77	0.47
1:R:275:SER:O	1:R:276:GLU:C	2.52	0.47
1:B:118:THR:HG23	1:B:121:GLU:N	2.21	0.47
1:B:87:ASP:CG	1:B:87:ASP:O	2.47	0.47
1:D:192:PRO:HD3	3:D:520:HOH:O	2.13	0.47
1:F:276:GLU:OE2	1:F:307:ALA:HB3	2.14	0.47
1:G:197:ASP:HA	1:G:235:ALA:HB1	1.96	0.47
1:J:342:TYR:OH	1:J:345:THR:HA	2.15	0.47
1:L:201:CYS:SG	1:L:233:VAL:HG13	2.54	0.47
1:O:329:LYS:O	1:O:330:ARG:C	2.52	0.47
1:P:75:GLY:HA2	1:P:103:VAL:O	2.15	0.47
1:Q:68:SER:O	1:Q:71:GLN:HB2	2.14	0.47
1:A:18:ILE:HD13	1:A:143:ASP:HB3	1.97	0.47
1:B:326:ALA:O	1:B:329:LYS:HB3	2.14	0.47
1:B:6:ALA:HB3	3:B:419:HOH:O	2.13	0.47
1:C:285:ALA:O	1:C:286:ILE:C	2.53	0.47
1:D:118:THR:CG2	1:D:121:GLU:HB2	2.44	0.47
1:D:330:ARG:HH11	1:D:347:SER:CB	2.28	0.47
1:D:330:ARG:HH11	1:D:347:SER:HB2	1.79	0.47
1:E:320:LYS:HE3	1:E:324:GLN:NE2	2.30	0.47
1:I:18:ILE:HD13	1:I:143:ASP:HB3	1.97	0.47
1:I:39:MET:O	1:I:40:GLY:C	2.53	0.47
1:I:4:PHE:CZ	1:J:119:ASN:HB2	2.50	0.47
1:J:106:ILE:HG22	1:J:142:VAL:HG11	1.97	0.47
1:J:80:HIS:CD2	1:J:137:TYR:OH	2.68	0.47
1:M:226:THR:CG2	3:M:509:HOH:O	2.62	0.47
1:P:25:ASN:H	1:P:27:LYS:HB2	1.80	0.47
1:A:67:SER:C	1:A:69:ILE:H	2.17	0.46
1:B:207:LYS:HE2	1:C:2:HIS:NE2	2.29	0.46
1:C:343:VAL:HG12	1:C:344:HIS:N	2.30	0.46
1:D:250:MET:HE3	1:D:254:THR:OG1	2.16	0.46
1:E:33:ASP:N	1:E:33:ASP:OD1	2.48	0.46
1:F:27:LYS:HE2	3:F:424:HOH:O	2.15	0.46
1:I:276:GLU:HG2	1:I:304:ALA:O	2.15	0.46
1:M:68:SER:HA	1:M:69:ILE:CG1	2.26	0.46
1:N:65:VAL:O	1:N:66:ASP:C	2.52	0.46
1:Q:231:ASN:ND2	1:Q:231:ASN:H	2.12	0.46
1:R:198:LEU:HD12	1:R:234:THR:HA	1.97	0.46
1:A:220:HIS:CE1	3:A:559:HOH:O	2.58	0.46
1:C:128:ASP:OD2	1:D:128:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:ILE:HG21	1:F:29:ILE:HD13	1.44	0.46
1:G:113:ALA:HA	1:G:114:PRO:HD2	1.60	0.46
1:H:202:GLN:HB2	1:H:233:VAL:HG11	1.96	0.46
1:J:230:PRO:CG	1:J:267:ILE:CD1	2.91	0.46
1:K:277:GLU:OE2	1:K:344:HIS:HD2	1.97	0.46
1:M:349:GLY:O	1:M:350:ALA:CB	2.63	0.46
1:N:173:TYR:CE1	1:N:177:CYS:SG	3.08	0.46
1:O:159:SER:HB3	1:P:1:ALA:HA	1.97	0.46
1:O:321:GLU:O	1:O:322:ALA:C	2.53	0.46
1:P:44:GLN:HA	1:P:44:GLN:OE1	2.13	0.46
1:Q:156:GLN:NE2	1:R:3:ARG:CD	2.76	0.46
1:A:256:LEU:CD1	1:A:267:ILE:HD11	2.46	0.46
1:A:345:THR:O	1:A:346:GLY:C	2.50	0.46
1:A:69:ILE:HD12	1:A:327:PHE:CE2	2.51	0.46
1:C:36:VAL:HG13	1:C:55:ARG:CZ	2.45	0.46
1:F:191:ILE:HD12	1:F:191:ILE:HA	1.59	0.46
1:G:124:ILE:HG22	1:G:147:TRP:CZ2	2.51	0.46
1:G:44:GLN:O	1:G:45:ARG:C	2.52	0.46
1:H:12:LYS:HE2	1:H:222:TYR:CD1	2.50	0.46
1:H:224:GLU:HG3	1:H:263:ALA:HB1	1.97	0.46
1:N:83:LEU:O	1:N:83:LEU:HG	2.15	0.46
1:O:48:VAL:HG21	1:O:315:GLY:HA3	1.97	0.46
1:P:196:HIS:O	1:P:239:CYS:HB2	2.16	0.46
1:P:252:THR:O	1:P:256:LEU:HG	2.15	0.46
1:B:243:TYR:HA	1:B:247:GLN:OE1	2.15	0.46
1:E:61:ILE:CG2	1:E:324:GLN:HG2	2.45	0.46
1:G:119:ASN:HB2	1:H:4:PHE:CZ	2.51	0.46
1:H:29:ILE:HD13	1:H:29:ILE:HG21	1.77	0.46
1:M:115:LEU:HD22	1:M:122:THR:C	2.36	0.46
1:M:29:ILE:HB	1:M:300:SER:HA	1.98	0.46
1:M:156:GLN:CD	1:N:2:HIS:HB3	2.36	0.46
1:D:106:ILE:HD12	1:D:107:LYS:N	2.31	0.46
1:F:105:GLY:HA2	1:F:144:PHE:O	2.15	0.46
1:F:270:LEU:O	1:F:270:LEU:HD12	2.15	0.46
1:F:276:GLU:CB	1:F:352:SER:HB3	2.46	0.46
1:H:115:LEU:HD13	1:H:123:THR:OG1	2.16	0.46
1:H:198:LEU:CD1	1:H:234:THR:HA	2.46	0.46
1:I:224:GLU:HG2	3:I:422:HOH:O	2.16	0.46
1:I:51:THR:HG22	1:I:53:GLU:CA	2.44	0.46
1:J:244:THR:HG23	1:J:246:GLU:OE1	2.15	0.46
1:J:71:GLN:CG	3:J:504:HOH:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:ILE:HD13	1:M:29:ILE:HG21	1.65	0.46
1:M:43:LEU:O	1:M:44:GLN:C	2.52	0.46
1:M:69:ILE:HG23	1:M:69:ILE:H	1.44	0.46
1:M:8:THR:OG1	1:M:11:GLN:HG3	2.14	0.46
1:N:41:ASN:O	1:N:44:GLN:HB3	2.16	0.46
1:P:270:LEU:HD12	1:P:270:LEU:O	2.16	0.46
1:A:277:GLU:OE1	1:A:347:SER:HB2	2.16	0.46
1:A:45:ARG:NH1	1:A:357:PHE:HA	2.27	0.46
1:A:51:THR:CG2	1:A:54:ASN:N	2.59	0.46
1:B:281:LEU:HD21	1:B:344:HIS:CE1	2.49	0.46
1:C:189:GLU:HB2	1:C:270:LEU:CD2	2.46	0.46
1:C:284:ASN:OD1	1:C:340:GLY:HA2	2.15	0.46
1:J:185:ILE:HD13	1:J:185:ILE:HG21	1.72	0.46
1:J:244:THR:HG23	1:J:246:GLU:N	2.31	0.46
1:K:12:LYS:O	1:K:13:LYS:C	2.52	0.46
1:L:313:TRP:CH2	1:L:315:GLY:HA2	2.50	0.46
1:M:124:ILE:HG21	1:M:147:TRP:CE2	2.51	0.46
1:M:256:LEU:HD13	1:M:267:ILE:HD13	1.98	0.46
1:M:267:ILE:HG21	1:M:267:ILE:HD13	1.69	0.46
1:M:312:ALA:O	1:M:319:ASN:HB3	2.16	0.46
1:M:3:ARG:CZ	1:N:156:GLN:HE22	2.28	0.46
1:O:173:TYR:CE1	1:O:177:CYS:SG	3.09	0.46
1:P:2:HIS:O	1:P:3:ARG:O	2.33	0.46
1:A:87:ASP:HB2	1:A:91:LYS:O	2.16	0.46
1:B:136:GLN:O	1:B:140:ASP:N	2.46	0.46
1:C:159:SER:HB2	1:D:1:ALA:HB2	1.94	0.46
1:C:189:GLU:CG	1:C:191:ILE:CD1	2.94	0.46
1:D:250:MET:CE	1:D:291:LEU:CD2	2.94	0.46
1:L:49:GLU:O	1:L:51:THR:N	2.48	0.46
1:M:106:ILE:O	1:M:145:GLY:HA2	2.16	0.46
1:M:123:THR:HG21	1:M:165:GLU:OE2	2.16	0.46
1:M:277:GLU:OE2	1:M:342:TYR:OH	2.27	0.46
1:M:329:LYS:HZ1	1:M:348:SER:CB	2.28	0.46
1:M:66:ASP:C	1:M:68:SER:N	2.58	0.46
1:C:34:GLU:HB3	1:C:38:THR:HB	1.97	0.46
1:C:51:THR:O	1:C:51:THR:HG22	2.15	0.46
1:D:270:LEU:C	1:D:270:LEU:HD12	2.36	0.46
1:E:51:THR:O	1:E:52:GLU:C	2.53	0.46
1:F:92:LEU:O	1:F:95:ASN:N	2.47	0.46
1:G:250:MET:HE1	1:G:291:LEU:HD21	1.98	0.46
1:G:62:LEU:O	1:G:65:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:ILE:HA	1:H:192:PRO:HD3	1.84	0.46
1:H:51:THR:HG22	1:H:51:THR:O	2.16	0.46
1:I:250:MET:CE	1:I:291:LEU:CD2	2.94	0.46
1:I:67:SER:OG	1:I:68:SER:N	2.10	0.46
1:J:329:LYS:CE	1:J:346:GLY:O	2.63	0.46
1:L:284:ASN:O	1:L:285:ALA:C	2.54	0.46
1:M:329:LYS:CE	1:M:347:SER:CB	2.86	0.46
1:N:244:THR:HG23	1:N:247:GLN:H	1.75	0.46
1:O:78:LEU:O	1:O:106:ILE:HD12	2.16	0.46
1:P:118:THR:HG23	1:P:121:GLU:H	1.81	0.46
1:P:154:ALA:HB3	1:P:157:CYS:HB2	1.96	0.46
1:M:2:HIS:HE2	1:P:207:LYS:HE2	1.81	0.46
1:Q:58:PHE:CE2	1:Q:310:LEU:HD13	2.51	0.46
1:R:172:ARG:NH2	1:R:176:ILE:HD11	2.30	0.46
1:A:231:ASN:H	1:A:231:ASN:ND2	2.14	0.46
1:C:263:ALA:O	1:C:265:PRO:HD3	2.15	0.46
1:D:250:MET:HE3	1:D:291:LEU:HD21	1.97	0.46
1:D:27:LYS:HB3	1:D:72:SER:O	2.15	0.46
1:E:146:LYS:HE2	1:E:187:GLU:OE1	2.15	0.46
1:E:65:VAL:HG21	1:E:69:ILE:HG12	1.97	0.46
1:G:50:ASN:HD21	1:G:55:ARG:HD3	1.81	0.46
1:H:276:GLU:OE2	1:H:307:ALA:HB3	2.15	0.46
1:I:156:GLN:O	1:J:1:ALA:HB1	2.16	0.46
1:I:244:THR:HG22	1:I:247:GLN:HB2	1.97	0.46
1:I:87:ASP:OD1	1:I:89:GLN:HB3	2.15	0.46
1:K:116:ALA:N	3:K:501:HOH:O	2.43	0.46
1:O:230:PRO:CG	1:O:267:ILE:HD13	2.46	0.46
1:P:106:ILE:HD12	1:P:106:ILE:HA	1.61	0.46
1:P:294:PRO:HG2	1:P:295:TRP:CE2	2.51	0.46
1:R:220:HIS:HE1	3:R:523:HOH:O	1.97	0.46
1:B:51:THR:CG2	1:B:54:ASN:N	2.59	0.46
1:C:325:GLU:O	1:C:328:MET:HB3	2.16	0.46
1:C:83:LEU:HG	1:C:83:LEU:O	2.16	0.46
1:D:106:ILE:HD12	1:D:107:LYS:H	1.81	0.46
1:G:172:ARG:NH2	1:G:176:ILE:HD11	2.31	0.46
1:G:55:ARG:NE	1:G:81:GLU:OE2	2.39	0.46
1:I:326:ALA:O	1:I:327:PHE:C	2.49	0.46
1:J:252:THR:O	1:J:256:LEU:HG	2.16	0.46
1:K:244:THR:HG23	1:K:246:GLU:HB2	1.97	0.46
1:L:160:SER:O	1:L:161:LEU:C	2.52	0.46
1:L:29:ILE:HB	1:L:300:SER:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:ASN:HB2	1:L:4:PHE:CD1	2.51	0.46
1:M:160:SER:O	1:M:164:GLN:HB3	2.16	0.46
1:M:279:ALA:HB1	1:M:301:TYR:CZ	2.52	0.46
1:P:119:ASN:O	1:P:119:ASN:CG	2.53	0.46
1:B:191:ILE:HD12	1:B:191:ILE:HG23	1.68	0.45
1:C:1:ALA:N	1:D:121:GLU:OE1	2.49	0.45
1:D:121:GLU:OE2	1:D:158:PRO:HA	2.15	0.45
1:D:279:ALA:HB1	1:D:301:TYR:CE1	2.52	0.45
1:D:87:ASP:HB2	1:D:91:LYS:O	2.17	0.45
1:F:58:PHE:CE2	1:F:62:LEU:HD11	2.51	0.45
1:G:271:SER:HB3	1:G:301:TYR:CD2	2.51	0.45
1:I:211:ALA:O	1:I:212:VAL:C	2.52	0.45
1:J:217:ASN:OD1	3:J:502:HOH:O	2.21	0.45
1:J:87:ASP:HB2	1:J:88:SER:H	1.45	0.45
1:L:46:ILE:HD12	1:L:48:VAL:CG2	2.46	0.45
1:N:244:THR:O	1:N:247:GLN:N	2.48	0.45
1:N:335:CYS:O	1:N:339:LYS:HG3	2.15	0.45
1:P:103:VAL:CG1	1:P:143:ASP:HB2	2.45	0.45
1:P:83:LEU:HD23	1:P:84:TYR:CE1	2.51	0.45
1:R:121:GLU:OE1	1:R:159:SER:CB	2.64	0.45
1:A:50:ASN:ND2	1:A:50:ASN:C	2.67	0.45
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.98	0.45
1:B:226:THR:CG2	1:B:227:LEU:N	2.80	0.45
1:B:70:ASN:C	1:B:70:ASN:OD1	2.55	0.45
1:C:289:CYS:O	1:C:293:LYS:NZ	2.41	0.45
1:D:250:MET:HE3	1:D:254:THR:HG1	1.80	0.45
1:E:129:GLY:HA2	1:E:132:GLU:OE1	2.16	0.45
1:G:1:ALA:O	1:G:2:HIS:HB2	2.17	0.45
1:H:244:THR:HB	1:H:245:PRO:HD2	1.98	0.45
1:I:78:LEU:O	1:I:106:ILE:HA	2.16	0.45
1:I:231:ASN:HA	1:I:270:LEU:HG	1.98	0.45
1:I:337:ALA:C	1:I:339:LYS:N	2.68	0.45
1:I:67:SER:HB3	1:I:69:ILE:H	1.82	0.45
1:K:170:LEU:HD22	1:K:186:VAL:HG13	1.98	0.45
1:L:271:SER:HA	1:L:274:MET:CE	2.46	0.45
1:N:51:THR:O	1:N:51:THR:HG22	2.16	0.45
1:Q:226:THR:HG23	3:Q:2024:HOH:O	2.09	0.45
1:Q:319:ASN:N	1:Q:319:ASN:OD1	2.46	0.45
1:R:80:HIS:CD2	1:R:137:TYR:OH	2.65	0.45
1:R:172:ARG:HH11	1:R:172:ARG:HD2	1.53	0.45
1:A:65:VAL:HG23	1:A:324:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG23	1:A:53:GLU:N	2.32	0.45
1:A:83:LEU:HD23	1:A:84:TYR:CE1	2.51	0.45
1:A:87:ASP:HB2	1:A:91:LYS:H	1.80	0.45
1:A:87:ASP:OD2	1:A:91:LYS:HB3	2.16	0.45
1:B:25:ASN:H	1:B:27:LYS:HG3	1.81	0.45
1:G:12:LYS:HD3	1:G:222:TYR:CE1	2.51	0.45
1:G:2:HIS:HB3	1:H:156:GLN:OE1	2.17	0.45
1:H:348:SER:HB3	1:H:349:GLY:H	1.61	0.45
1:H:60:GLU:OE1	1:H:87:ASP:HB2	2.16	0.45
1:K:222:TYR:O	1:K:223:LEU:C	2.54	0.45
1:M:68:SER:O	1:M:69:ILE:CB	2.44	0.45
1:O:303:ARG:HH11	1:O:303:ARG:HG3	1.81	0.45
1:O:61:ILE:HG12	1:O:320:LYS:HG3	1.99	0.45
1:P:81:GLU:HG2	1:P:82:THR:N	2.31	0.45
1:Q:313:TRP:CD2	1:Q:315:GLY:HA2	2.51	0.45
1:A:3:ARG:HH21	1:B:156:GLN:NE2	2.15	0.45
1:C:144:PHE:HB2	1:C:183:VAL:O	2.16	0.45
1:D:244:THR:CG2	1:D:246:GLU:H	2.27	0.45
1:D:89:GLN:HE21	1:D:89:GLN:HB2	1.53	0.45
1:H:354:GLN:HG3	1:H:356:LEU:HD23	1.98	0.45
1:I:58:PHE:CE1	1:I:310:LEU:CD1	3.00	0.45
1:J:144:PHE:HB2	1:J:183:VAL:O	2.16	0.45
1:J:320:LYS:O	1:J:324:GLN:HG3	2.16	0.45
1:M:189:GLU:HG2	1:M:191:ILE:CD1	2.47	0.45
1:M:277:GLU:O	1:M:278:ASP:C	2.50	0.45
1:M:276:GLU:OE2	1:M:307:ALA:HB3	2.15	0.45
1:N:50:ASN:HD21	1:N:55:ARG:HH11	1.60	0.45
1:Q:217:ASN:C	1:Q:217:ASN:ND2	2.70	0.45
1:F:118:THR:HG23	1:F:121:GLU:H	1.81	0.45
1:I:14:GLU:O	1:I:18:ILE:HG13	2.16	0.45
1:J:296:LYS:HA	1:J:296:LYS:HD2	1.74	0.45
1:L:144:PHE:HB2	1:L:183:VAL:O	2.17	0.45
1:M:329:LYS:HD2	1:M:347:SER:CB	2.46	0.45
1:O:8:THR:OG1	1:O:11:GLN:HG3	2.16	0.45
1:O:28:GLY:HA3	1:O:299:PHE:CZ	2.51	0.45
1:P:109:ASP:HB3	1:P:147:TRP:HA	1.99	0.45
1:P:51:THR:HG22	1:P:54:ASN:HB2	1.98	0.45
1:P:91:LYS:HD3	1:P:96:ILE:CG1	2.47	0.45
1:Q:115:LEU:HA	1:Q:115:LEU:HD12	1.80	0.45
1:Q:152:ARG:HH11	1:Q:152:ARG:HD3	1.36	0.45
1:R:276:GLU:HB3	3:R:515:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:HG21	3:A:536:HOH:O	2.09	0.45
1:B:136:GLN:HB2	1:B:136:GLN:HE21	1.52	0.45
1:B:244:THR:O	1:B:244:THR:HG22	2.17	0.45
1:B:313:TRP:CH2	1:B:315:GLY:HA2	2.52	0.45
1:E:191:ILE:HG21	1:E:191:ILE:HD13	1.25	0.45
1:F:343:VAL:O	1:F:344:HIS:C	2.55	0.45
1:G:244:THR:CG2	1:G:247:GLN:N	2.79	0.45
1:G:69:ILE:O	1:G:71:GLN:N	2.49	0.45
1:I:176:ILE:O	1:I:177:CYS:C	2.55	0.45
1:J:3:ARG:HB2	1:J:4:PHE:H	1.74	0.45
1:K:128:ASP:HA	1:L:125:GLN:NE2	2.32	0.45
1:K:335:CYS:SG	1:K:339:LYS:NZ	2.90	0.45
1:L:119:ASN:HB3	1:L:157:CYS:SG	2.56	0.45
1:L:2:HIS:HB3	1:L:3:ARG:H	1.54	0.45
1:M:222:TYR:CZ	1:M:224:GLU:HG2	2.51	0.45
1:N:284:ASN:ND2	1:N:340:GLY:CA	2.80	0.45
1:N:28:GLY:HA3	1:N:299:PHE:CE1	2.52	0.45
1:O:343:VAL:CG2	1:O:344:HIS:H	2.10	0.45
1:O:79:PHE:O	1:O:80:HIS:C	2.55	0.45
1:P:276:GLU:CG	1:P:352:SER:HB2	2.47	0.45
1:Q:118:THR:CG2	1:Q:121:GLU:HB2	2.46	0.45
1:A:2:HIS:HA	1:D:203:TYR:OH	2.15	0.45
1:B:279:ALA:HB1	1:B:301:TYR:CZ	2.51	0.45
1:C:106:ILE:HG23	1:C:106:ILE:O	2.15	0.45
1:A:224:GLU:OE2	1:D:258:ARG:HD3	2.16	0.45
1:F:171:ALA:HA	1:F:216:LEU:HD12	1.98	0.45
1:F:352:SER:HA	1:F:354:GLN:CB	2.47	0.45
1:L:66:ASP:O	1:L:67:SER:C	2.53	0.45
1:M:119:ASN:H	1:N:1:ALA:CB	2.27	0.45
1:M:351:ALA:O	1:M:352:SER:HB2	2.16	0.45
1:O:87:ASP:OD2	1:O:91:LYS:N	2.45	0.45
1:P:86:LYS:HD3	1:P:90:GLY:HA2	1.99	0.45
1:Q:254:THR:O	1:Q:258:ARG:HG2	2.17	0.45
1:A:276:GLU:HG2	1:A:304:ALA:O	2.17	0.45
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.60	0.45
1:B:119:ASN:HB3	1:B:157:CYS:SG	2.56	0.45
1:B:59:ARG:O	1:B:63:PHE:N	2.39	0.45
1:C:36:VAL:CG1	1:C:36:VAL:O	2.64	0.45
1:D:118:THR:HG23	1:D:121:GLU:HB2	1.97	0.45
1:E:75:GLY:HA2	1:E:103:VAL:O	2.17	0.45
1:F:274:MET:HE3	1:F:279:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:ILE:CG1	1:F:297:LEU:HD23	2.41	0.45
1:H:187:GLU:HG3	1:H:229:LYS:HG2	1.99	0.45
1:I:38:THR:O	1:I:39:MET:C	2.55	0.45
1:N:284:ASN:HD22	1:N:340:GLY:CA	2.26	0.45
1:O:320:LYS:O	1:O:323:THR:HB	2.17	0.45
1:P:23:VAL:CG2	1:P:296:LYS:HG3	2.47	0.45
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.99	0.45
1:B:76:VAL:HG23	1:B:102:ILE:HG21	1.99	0.45
1:G:184:PRO:HD2	1:G:225:GLY:O	2.17	0.45
1:G:51:THR:CG2	1:G:54:ASN:N	2.72	0.45
1:I:12:LYS:HG2	1:I:222:TYR:CD1	2.52	0.45
1:J:227:LEU:HA	1:J:227:LEU:HD23	1.72	0.45
1:J:354:GLN:HB3	3:J:501:HOH:O	2.17	0.45
1:K:172:ARG:HH11	1:K:172:ARG:HD2	1.50	0.45
1:L:83:LEU:HB3	1:L:84:TYR:CD1	2.52	0.45
1:M:352:SER:HA	1:M:354:GLN:N	2.32	0.45
1:N:83:LEU:HD23	1:N:84:TYR:CE1	2.52	0.45
1:O:244:THR:O	1:O:245:PRO:C	2.56	0.45
1:O:65:VAL:HB	1:O:328:MET:CE	2.47	0.45
1:O:61:ILE:HG22	1:O:324:GLN:HG2	1.99	0.45
1:Q:289:CYS:SG	1:Q:291:LEU:HD22	2.57	0.45
1:A:80:HIS:CD2	1:A:137:TYR:OH	2.68	0.45
1:A:229:LYS:HZ2	1:A:300:SER:CB	2.29	0.45
1:B:108:LEU:HB3	1:B:130:LEU:HD11	2.00	0.45
1:B:44:GLN:O	1:B:45:ARG:C	2.53	0.45
1:B:95:ASN:O	1:B:96:ILE:C	2.54	0.45
1:C:121:GLU:OE2	1:C:157:CYS:HB3	2.17	0.45
1:E:223:LEU:HD11	3:E:555:HOH:O	2.17	0.45
1:F:118:THR:HG23	1:F:121:GLU:CB	2.40	0.45
1:J:226:THR:CG2	3:J:511:HOH:O	2.65	0.45
1:K:154:ALA:O	1:K:155:ASP:C	2.55	0.45
1:M:119:ASN:OD1	1:M:119:ASN:C	2.56	0.45
1:N:3:ARG:N	1:N:3:ARG:HH11	2.14	0.45
1:P:80:HIS:CD2	1:P:137:TYR:OH	2.58	0.45
1:P:330:ARG:HD3	1:P:330:ARG:HH11	0.92	0.45
1:R:245:PRO:HD2	1:R:246:GLU:OE1	2.17	0.45
1:A:123:THR:CG2	1:A:124:ILE:H	2.30	0.44
1:B:75:GLY:HA2	1:B:103:VAL:O	2.16	0.44
1:E:250:MET:HE3	1:E:291:LEU:HD22	1.92	0.44
1:F:50:ASN:HD22	1:F:51:THR:N	2.15	0.44
1:L:95:ASN:O	1:L:96:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:THR:O	1:N:242:LYS:HE3	2.17	0.44
1:O:86:LYS:HA	1:O:91:LYS:O	2.17	0.44
1:Q:191:ILE:HA	1:Q:191:ILE:HD13	1.46	0.44
1:B:49:GLU:O	1:B:54:ASN:ND2	2.25	0.44
1:B:56:ARG:NH1	1:B:56:ARG:HG2	2.31	0.44
1:C:189:GLU:CD	1:C:191:ILE:CD1	2.85	0.44
1:C:41:ASN:O	1:C:44:GLN:HB3	2.18	0.44
1:C:94:ARG:HD3	1:C:140:ASP:O	2.16	0.44
1:D:329:LYS:HZ3	1:D:347:SER:CA	2.27	0.44
1:E:44:GLN:HA	1:E:44:GLN:OE1	2.17	0.44
1:F:58:PHE:CE1	1:F:310:LEU:CD1	3.00	0.44
1:G:119:ASN:C	1:G:119:ASN:OD1	2.53	0.44
1:G:65:VAL:CG1	1:G:324:GLN:HB3	2.47	0.44
1:H:12:LYS:HB3	1:H:222:TYR:CZ	2.52	0.44
1:H:277:GLU:HG2	1:H:345:THR:CG2	2.40	0.44
1:H:342:TYR:OH	1:H:346:GLY:N	2.51	0.44
1:H:61:ILE:CG2	1:H:324:GLN:HG2	2.48	0.44
1:J:86:LYS:HB3	1:J:90:GLY:HA2	1.99	0.44
1:K:355:SER:O	1:K:356:LEU:HD23	2.17	0.44
1:L:76:VAL:HG23	1:L:102:ILE:HG21	1.98	0.44
1:L:61:ILE:CG2	1:L:324:GLN:HG2	2.47	0.44
1:M:75:GLY:HA2	1:M:103:VAL:O	2.17	0.44
1:M:189:GLU:CD	1:M:191:ILE:HD13	2.37	0.44
1:M:272:GLY:HA2	1:M:303:ARG:HH12	1.82	0.44
1:N:193:ASP:OD1	1:N:193:ASP:N	2.51	0.44
1:C:133:ARG:O	1:C:134:CYS:C	2.53	0.44
1:C:164:GLN:O	1:C:168:ASN:ND2	2.47	0.44
1:D:75:GLY:CA	1:D:103:VAL:O	2.65	0.44
1:D:12:LYS:HG2	1:D:222:TYR:CZ	2.52	0.44
1:F:224:GLU:HB3	3:F:425:HOH:O	2.16	0.44
1:F:313:TRP:CE2	1:F:315:GLY:HA2	2.52	0.44
1:H:250:MET:HE1	1:H:291:LEU:HD13	1.99	0.44
1:H:233:VAL:CG2	1:H:252:THR:HA	2.48	0.44
1:H:267:ILE:HG12	1:H:297:LEU:HD23	1.98	0.44
1:I:201:CYS:SG	1:I:233:VAL:HG13	2.57	0.44
1:J:12:LYS:HE2	1:J:222:TYR:CD1	2.53	0.44
1:L:159:SER:O	1:L:160:SER:C	2.55	0.44
1:L:80:HIS:HD2	1:L:137:TYR:OH	2.01	0.44
1:M:155:ASP:O	1:M:156:GLN:HB2	2.17	0.44
1:M:352:SER:HA	1:M:354:GLN:HB3	1.98	0.44
1:M:68:SER:CA	1:M:69:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HB	1:A:300:SER:HA	1.99	0.44
1:B:148:ARG:HA	1:B:187:GLU:HB3	2.00	0.44
1:C:35:SER:O	1:C:36:VAL:C	2.55	0.44
1:E:324:GLN:O	1:E:328:MET:HB2	2.18	0.44
1:E:125:GLN:HE21	1:F:128:ASP:HA	1.83	0.44
1:F:148:ARG:HD3	3:F:458:HOH:O	2.17	0.44
1:F:191:ILE:HA	1:F:192:PRO:HD3	1.71	0.44
1:G:29:ILE:HG21	1:G:29:ILE:HD13	1.71	0.44
1:G:2:HIS:HB3	1:H:156:GLN:CD	2.38	0.44
1:H:1:ALA:CB	1:H:4:PHE:CD1	3.01	0.44
1:J:24:ALA:HA	3:J:543:HOH:O	2.17	0.44
1:J:316:LYS:O	1:J:317:ALA:C	2.55	0.44
1:K:28:GLY:HA3	1:K:299:PHE:CE1	2.52	0.44
1:L:244:THR:O	1:L:247:GLN:HB2	2.18	0.44
1:M:2:HIS:O	1:M:3:ARG:O	2.35	0.44
1:M:29:ILE:O	1:M:300:SER:HA	2.17	0.44
1:N:22:ILE:HD11	1:N:144:PHE:CD2	2.53	0.44
1:N:274:MET:HE3	1:N:279:ALA:CA	2.44	0.44
1:R:196:HIS:O	1:R:239:CYS:HB2	2.18	0.44
1:A:12:LYS:HG2	1:A:222:TYR:CE2	2.52	0.44
1:A:40:GLY:HA2	1:A:50:ASN:HB2	1.98	0.44
1:B:257:HIS:CD2	1:C:263:ALA:HA	2.52	0.44
1:C:270:LEU:HD12	1:C:270:LEU:C	2.38	0.44
1:D:279:ALA:HB1	1:D:301:TYR:CZ	2.52	0.44
1:E:4:PHE:HA	1:E:5:PRO:HD2	1.77	0.44
1:F:250:MET:CE	1:F:291:LEU:CD2	2.95	0.44
1:G:80:HIS:CD2	1:G:137:TYR:OH	2.70	0.44
1:J:253:VAL:O	1:J:254:THR:C	2.55	0.44
1:J:350:ALA:O	1:J:351:ALA:C	2.55	0.44
1:J:62:LEU:O	1:J:65:VAL:HG13	2.17	0.44
1:M:190:VAL:H	1:M:231:ASN:ND2	2.16	0.44
1:N:184:PRO:O	1:N:184:PRO:HG2	2.18	0.44
1:O:296:LYS:N	1:O:296:LYS:HD2	2.32	0.44
1:D:4:PHE:HA	1:D:5:PRO:HD2	1.76	0.44
1:E:124:ILE:CG2	1:E:147:TRP:CZ2	2.99	0.44
1:E:163:ILE:HG22	1:E:164:GLN:N	2.31	0.44
1:I:214:LYS:HE3	1:I:218:ASP:OD1	2.17	0.44
1:I:69:ILE:HD11	1:I:327:PHE:CE2	2.52	0.44
1:J:120:LYS:HB2	1:J:152:ARG:NH1	2.33	0.44
1:J:352:SER:CA	3:J:503:HOH:O	2.64	0.44
1:O:44:GLN:OE1	1:O:44:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:133:ARG:HD3	1:P:133:ARG:HH11	1.27	0.44
1:Q:253:VAL:HG23	1:Q:286:ILE:HG23	1.98	0.44
1:R:313:TRP:CH2	1:R:315:GLY:HA2	2.52	0.44
1:R:50:ASN:HD21	1:R:55:ARG:HH11	1.64	0.44
1:B:7:LEU:HD21	1:B:178:GLN:HB3	1.99	0.44
1:B:186:VAL:O	1:B:228:LEU:HD12	2.18	0.44
1:B:271:SER:O	1:B:272:GLY:C	2.56	0.44
1:B:69:ILE:C	1:B:71:GLN:H	2.21	0.44
1:C:110:GLN:N	1:C:125:GLN:O	2.49	0.44
1:C:244:THR:O	1:C:247:GLN:HB2	2.18	0.44
1:E:115:LEU:HD12	1:E:115:LEU:HA	1.78	0.44
1:F:291:LEU:O	1:F:292:PRO:C	2.55	0.44
1:F:45:ARG:HH12	1:F:356:LEU:HA	1.82	0.44
1:I:202:GLN:HB2	1:I:233:VAL:HG11	2.00	0.44
1:I:51:THR:O	1:I:51:THR:HG22	2.18	0.44
1:I:51:THR:CG2	1:I:53:GLU:HB3	2.47	0.44
1:J:207:LYS:HD3	3:K:570:HOH:O	2.17	0.44
1:M:271:SER:HB3	1:M:301:TYR:CD2	2.53	0.44
1:N:244:THR:HG23	1:N:246:GLU:CA	2.47	0.44
1:P:23:VAL:HG23	1:P:296:LYS:HG3	1.99	0.44
1:R:51:THR:O	1:R:52:GLU:C	2.56	0.44
1:A:343:VAL:O	1:A:344:HIS:C	2.54	0.44
1:A:117:GLY:HA2	1:B:4:PHE:O	2.17	0.44
1:D:160:SER:O	1:D:161:LEU:C	2.56	0.44
1:D:252:THR:O	1:D:256:LEU:HG	2.18	0.44
1:E:309:ALA:O	1:E:323:THR:HG23	2.18	0.44
1:F:60:GLU:HG3	1:F:93:PHE:HE1	1.83	0.44
1:G:51:THR:HG22	1:G:54:ASN:N	2.28	0.44
1:I:164:GLN:O	1:I:168:ASN:N	2.50	0.44
1:I:66:ASP:OD1	1:I:67:SER:HB2	2.18	0.44
1:K:244:THR:HG22	1:K:247:GLN:CB	2.48	0.44
1:L:256:LEU:HD13	1:L:267:ILE:HD11	1.99	0.44
1:L:232:MET:SD	1:L:274:MET:CE	3.06	0.44
1:L:333:ALA:O	1:L:336:GLN:HB2	2.18	0.44
1:O:104:VAL:HG12	1:O:105:GLY:N	2.33	0.44
1:O:191:ILE:CD1	1:O:192:PRO:HD2	2.48	0.44
1:O:295:TRP:CD2	1:O:295:TRP:N	2.85	0.44
1:P:173:TYR:CD2	1:P:174:ALA:N	2.86	0.44
1:P:268:CYS:HB3	1:P:300:SER:HB2	1.98	0.44
1:B:296:LYS:HA	1:B:296:LYS:HD2	1.75	0.44
1:B:69:ILE:HB	1:B:328:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:HD12	1:C:191:ILE:HA	1.21	0.44
1:E:224:GLU:OE2	1:H:258:ARG:NH1	2.34	0.44
1:E:28:GLY:HA3	1:E:299:PHE:CE2	2.53	0.44
1:E:329:LYS:CD	1:E:347:SER:OG	2.61	0.44
1:F:244:THR:HG22	1:F:247:GLN:CG	2.48	0.44
1:G:137:TYR:O	1:G:138:LYS:C	2.53	0.44
1:I:337:ALA:C	1:I:339:LYS:H	2.21	0.44
1:J:191:ILE:HD13	1:J:192:PRO:HD3	2.00	0.44
1:J:244:THR:H	1:J:247:GLN:HE21	1.61	0.44
1:J:81:GLU:HG2	1:J:82:THR:N	2.32	0.44
1:K:119:ASN:O	1:K:120:LYS:HB2	2.18	0.44
1:L:191:ILE:HG22	1:L:193:ASP:H	1.82	0.44
1:L:53:GLU:OE2	1:L:57:GLN:HG3	2.17	0.44
1:N:148:ARG:HB2	1:N:187:GLU:OE1	2.18	0.44
1:N:189:GLU:HB2	1:N:270:LEU:CD2	2.48	0.44
1:N:276:GLU:HB3	1:N:330:ARG:HH11	1.83	0.44
1:N:28:GLY:HA3	1:N:299:PHE:CZ	2.53	0.44
1:A:277:GLU:CD	1:A:347:SER:CB	2.85	0.43
1:A:30:LEU:HB3	1:A:76:VAL:HG22	1.99	0.43
1:D:286:ILE:HG22	1:D:297:LEU:HD13	2.00	0.43
1:D:53:GLU:HG3	1:D:57:GLN:NE2	2.32	0.43
1:K:130:LEU:HA	1:K:130:LEU:HD12	1.77	0.43
1:M:81:GLU:HG2	1:M:82:THR:N	2.32	0.43
1:O:223:LEU:HD23	1:O:223:LEU:HA	1.70	0.43
1:R:8:THR:HG21	3:R:501:HOH:O	2.18	0.43
1:A:190:VAL:H	1:A:231:ASN:ND2	2.16	0.43
1:B:173:TYR:CE1	1:B:177:CYS:SG	3.10	0.43
1:C:106:ILE:HD12	1:C:106:ILE:HA	1.78	0.43
1:D:119:ASN:HB3	1:D:157:CYS:HG	1.82	0.43
1:I:44:GLN:O	1:I:47:LYS:N	2.48	0.43
1:K:118:THR:CG2	1:K:121:GLU:HB2	2.48	0.43
1:K:226:THR:HG21	3:K:512:HOH:O	2.11	0.43
1:K:313:TRP:CZ2	1:K:315:GLY:HA2	2.53	0.43
1:K:30:LEU:HD22	1:K:327:PHE:CZ	2.53	0.43
1:L:155:ASP:O	1:L:156:GLN:CB	2.56	0.43
1:P:244:THR:HG23	1:P:246:GLU:H	1.82	0.43
1:R:112:GLY:HA2	1:R:123:THR:O	2.18	0.43
1:B:70:ASN:ND2	1:B:100:LYS:O	2.40	0.43
1:B:274:MET:HE3	1:B:279:ALA:CB	2.46	0.43
1:B:330:ARG:NE	1:B:330:ARG:CA	2.72	0.43
1:D:343:VAL:O	1:D:345:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:PHE:CE2	1:I:310:LEU:HD13	2.54	0.43
1:J:108:LEU:HD12	1:J:145:GLY:HA3	2.00	0.43
1:J:233:VAL:CG2	1:J:252:THR:HA	2.47	0.43
1:J:61:ILE:HG21	1:J:323:THR:CG2	2.48	0.43
1:K:118:THR:HG21	1:K:121:GLU:HB2	2.00	0.43
1:K:357:PHE:H	1:O:139:LYS:HZ1	1.65	0.43
1:K:357:PHE:H	1:O:139:LYS:NZ	2.16	0.43
1:Q:244:THR:HG23	1:Q:246:GLU:H	1.82	0.43
1:R:267:ILE:HG21	1:R:267:ILE:HD13	1.43	0.43
1:A:163:ILE:O	1:A:164:GLN:C	2.57	0.43
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.18	0.43
1:A:45:ARG:CZ	1:A:357:PHE:CA	2.74	0.43
1:B:1:ALA:H3	1:B:220:HIS:CE1	2.36	0.43
1:B:38:THR:O	1:B:41:ASN:N	2.51	0.43
1:E:51:THR:HG23	1:E:54:ASN:H	1.79	0.43
1:F:25:ASN:N	1:F:27:LYS:H	2.16	0.43
1:G:118:THR:HG23	1:G:119:ASN:N	2.34	0.43
1:G:3:ARG:H	1:G:4:PHE:HD1	1.65	0.43
1:H:276:GLU:H	1:H:352:SER:HB3	1.83	0.43
1:I:124:ILE:CG2	1:I:147:TRP:CZ2	3.00	0.43
1:N:36:VAL:HG13	1:N:55:ARG:NH1	2.33	0.43
1:O:191:ILE:HD13	1:O:191:ILE:HA	1.26	0.43
1:Q:128:ASP:HA	1:R:125:GLN:HE21	1.83	0.43
1:Q:109:ASP:HB3	1:Q:147:TRP:CD2	2.53	0.43
1:A:244:THR:CG2	1:A:244:THR:O	2.65	0.43
1:B:8:THR:HG1	1:B:11:GLN:HG3	1.77	0.43
1:C:198:LEU:CD1	1:C:234:THR:HA	2.48	0.43
1:C:244:THR:N	1:C:247:GLN:OE1	2.40	0.43
1:C:303:ARG:NH1	1:C:303:ARG:HG3	2.25	0.43
1:D:69:ILE:HG13	1:D:69:ILE:O	2.17	0.43
1:E:94:ARG:HD2	1:E:140:ASP:O	2.18	0.43
1:H:275:SER:O	1:H:276:GLU:C	2.57	0.43
1:H:8:THR:HG22	1:H:10:GLU:N	2.19	0.43
1:J:119:ASN:C	1:J:119:ASN:OD1	2.56	0.43
1:L:158:PRO:CG	1:L:163:ILE:HD11	2.49	0.43
1:L:43:LEU:O	1:L:46:ILE:HG13	2.18	0.43
1:M:115:LEU:O	1:M:118:THR:CG2	2.66	0.43
1:M:1:ALA:HB3	1:N:119:ASN:CB	2.48	0.43
1:O:164:GLN:HG2	1:O:165:GLU:N	2.32	0.43
1:P:263:ALA:O	1:P:265:PRO:HD3	2.19	0.43
1:R:289:CYS:O	1:R:293:LYS:CE	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:GLN:HG3	1:F:126:GLY:HA2	2.01	0.43
1:F:12:LYS:HD3	1:F:222:TYR:CE1	2.53	0.43
1:F:330:ARG:NH1	3:F:411:HOH:O	2.47	0.43
1:H:42:ARG:NH1	1:H:303:ARG:HG3	2.33	0.43
1:I:270:LEU:HD12	1:I:271:SER:N	2.33	0.43
1:N:118:THR:CG2	1:N:121:GLU:N	2.78	0.43
1:M:119:ASN:N	1:N:1:ALA:HB3	2.27	0.43
1:Q:58:PHE:CE1	1:Q:310:LEU:HD13	2.54	0.43
1:Q:87:ASP:HB2	1:Q:91:LYS:N	2.34	0.43
1:A:3:ARG:CD	1:B:156:GLN:NE2	2.82	0.43
1:B:313:TRP:CD2	1:B:315:GLY:HA2	2.53	0.43
1:C:147:TRP:CB	1:C:173:TYR:CE2	3.02	0.43
1:F:233:VAL:CG2	1:F:252:THR:HA	2.49	0.43
1:G:3:ARG:O	1:G:4:PHE:C	2.57	0.43
1:I:4:PHE:O	1:J:117:GLY:HA2	2.19	0.43
1:J:33:ASP:HB3	1:J:77:ILE:HG22	2.00	0.43
1:K:115:LEU:HD22	1:K:122:THR:C	2.39	0.43
1:N:244:THR:HG21	1:N:247:GLN:HG3	1.96	0.43
1:O:121:GLU:OE2	1:O:158:PRO:HA	2.18	0.43
1:R:254:THR:HG21	2:R:402:SO4:O4	2.19	0.43
1:A:86:LYS:HD3	1:A:90:GLY:HA2	2.01	0.43
1:B:285:ALA:O	1:B:286:ILE:C	2.55	0.43
1:C:172:ARG:HH11	1:C:172:ARG:HD2	1.54	0.43
1:C:147:TRP:CB	1:C:173:TYR:CZ	3.02	0.43
1:C:66:ASP:O	1:C:68:SER:N	2.52	0.43
1:D:121:GLU:HG3	1:D:157:CYS:SG	2.59	0.43
1:D:329:LYS:CD	1:D:347:SER:N	2.81	0.43
1:E:160:SER:O	1:E:161:LEU:C	2.56	0.43
1:E:46:ILE:O	1:E:48:VAL:HG23	2.18	0.43
1:F:195:ASP:HB3	1:F:238:ALA:CB	2.48	0.43
1:G:46:ILE:HG13	1:G:48:VAL:HG23	2.01	0.43
1:H:250:MET:HE1	1:H:291:LEU:CD1	2.49	0.43
1:J:193:ASP:OD1	1:J:193:ASP:N	2.52	0.43
1:L:65:VAL:HG23	1:L:69:ILE:HB	2.01	0.43
1:M:229:LYS:HA	1:M:268:CYS:O	2.19	0.43
1:M:68:SER:C	1:M:70:ASN:N	2.46	0.43
1:N:147:TRP:HB3	1:N:173:TYR:CE2	2.54	0.43
1:N:39:MET:O	1:N:40:GLY:C	2.55	0.43
1:N:60:GLU:HB2	1:N:93:PHE:CZ	2.53	0.43
1:O:201:CYS:O	1:O:202:GLN:C	2.57	0.43
1:P:146:LYS:CE	3:P:557:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:191:ILE:HD13	1:P:191:ILE:HA	1.68	0.43
1:P:223:LEU:HD23	1:P:223:LEU:HA	1.74	0.43
1:R:12:LYS:HB3	1:R:222:TYR:CZ	2.53	0.43
1:R:191:ILE:HG21	1:R:191:ILE:HD13	1.32	0.43
1:B:184:PRO:HD2	1:B:225:GLY:O	2.18	0.43
1:B:224:GLU:OE2	1:C:258:ARG:NH1	2.43	0.43
1:D:44:GLN:O	1:D:45:ARG:C	2.54	0.43
1:E:184:PRO:HD2	1:E:225:GLY:O	2.19	0.43
1:E:267:ILE:HG23	1:E:267:ILE:HD13	1.75	0.43
1:G:190:VAL:H	1:G:231:ASN:HD22	1.65	0.43
1:H:29:ILE:HB	1:H:300:SER:HA	2.00	0.43
1:H:329:LYS:HE2	1:H:347:SER:HA	2.00	0.43
1:I:337:ALA:O	1:I:339:LYS:N	2.52	0.43
1:J:235:ALA:HB2	1:J:243:TYR:CE1	2.54	0.43
1:K:61:ILE:HG12	1:K:320:LYS:HG3	2.00	0.43
1:M:128:ASP:OD2	1:N:128:ASP:N	2.36	0.43
1:M:187:GLU:HG2	1:M:187:GLU:O	2.19	0.43
1:N:285:ALA:O	1:N:286:ILE:C	2.55	0.43
1:P:184:PRO:HD2	1:P:225:GLY:O	2.18	0.43
1:A:14:GLU:O	1:A:18:ILE:HG13	2.19	0.43
1:A:254:THR:HG21	2:A:402:SO4:O3	2.19	0.43
1:D:259:THR:O	1:D:261:PRO:HD3	2.19	0.43
1:E:352:SER:HA	1:E:354:GLN:HG2	2.01	0.43
1:F:250:MET:HE3	1:F:291:LEU:CD2	2.48	0.43
1:F:252:THR:O	1:F:256:LEU:HG	2.19	0.43
1:H:80:HIS:CD2	1:H:137:TYR:OH	2.60	0.43
1:H:299:PHE:HB2	1:H:301:TYR:CD1	2.53	0.43
1:H:3:ARG:HB3	1:H:4:PHE:CD1	2.54	0.43
1:I:109:ASP:HA	1:I:147:TRP:CE3	2.53	0.43
1:I:115:LEU:HD11	1:I:165:GLU:HG2	2.00	0.43
1:I:2:HIS:HA	1:L:203:TYR:OH	2.19	0.43
1:J:105:GLY:HA2	1:J:144:PHE:O	2.19	0.43
1:J:229:LYS:HA	1:J:268:CYS:O	2.19	0.43
1:L:107:LYS:HE2	1:L:107:LYS:HB2	1.96	0.43
1:L:28:GLY:HA3	1:L:299:PHE:CZ	2.54	0.43
1:L:46:ILE:HG21	1:L:310:LEU:O	2.19	0.43
1:M:124:ILE:CG2	1:M:147:TRP:CE2	3.01	0.43
1:M:1:ALA:HB1	1:N:156:GLN:CB	2.48	0.43
1:N:3:ARG:HD2	1:N:220:HIS:CD2	2.54	0.43
1:P:330:ARG:NH1	3:P:506:HOH:O	2.50	0.43
1:Q:244:THR:CG2	1:Q:247:GLN:N	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB3	1:A:188:PRO:HA	2.00	0.42
1:A:256:LEU:HD13	1:A:267:ILE:CD1	2.49	0.42
1:B:118:THR:HG23	1:B:121:GLU:HG3	2.00	0.42
1:B:106:ILE:CG2	1:B:142:VAL:HG11	2.48	0.42
1:B:88:SER:O	1:B:89:GLN:CB	2.62	0.42
1:C:128:ASP:HB2	1:D:128:ASP:OD2	2.19	0.42
1:D:163:ILE:O	1:D:164:GLN:C	2.55	0.42
1:D:82:THR:HG21	3:D:529:HOH:O	2.19	0.42
1:F:214:LYS:HG3	1:F:214:LYS:O	2.19	0.42
1:G:123:THR:CG2	1:G:165:GLU:HG3	2.43	0.42
1:I:60:GLU:OE1	1:I:87:ASP:HB2	2.18	0.42
1:J:191:ILE:HA	1:J:192:PRO:HD3	1.83	0.42
1:J:28:GLY:HA3	1:J:299:PHE:CE2	2.54	0.42
1:K:344:HIS:CE1	1:K:348:SER:HB2	2.54	0.42
1:K:88:SER:O	1:K:89:GLN:HG2	2.16	0.42
1:M:98:LYS:HE3	1:M:141:GLY:HA3	2.01	0.42
1:N:123:THR:HG21	1:N:165:GLU:OE2	2.18	0.42
1:O:226:THR:HG23	1:O:227:LEU:N	2.34	0.42
1:P:224:GLU:OE1	1:P:224:GLU:N	2.47	0.42
1:Q:217:ASN:C	1:Q:217:ASN:HD22	2.23	0.42
1:A:298:SER:OG	1:A:299:PHE:N	2.50	0.42
1:B:58:PHE:CD1	1:B:310:LEU:CD1	3.02	0.42
1:C:330:ARG:HA	1:C:330:ARG:NE	2.34	0.42
1:D:267:ILE:HG21	1:D:267:ILE:HD13	1.57	0.42
1:D:350:ALA:O	1:D:354:GLN:N	2.52	0.42
1:E:88:SER:C	1:E:89:GLN:NE2	2.72	0.42
1:G:123:THR:O	1:G:124:ILE:HD12	2.19	0.42
1:G:148:ARG:HD2	3:G:516:HOH:O	2.19	0.42
1:G:148:ARG:HA	1:G:187:GLU:HB3	2.01	0.42
1:H:303:ARG:HB3	1:H:356:LEU:CD1	2.49	0.42
1:I:17:GLU:O	1:I:18:ILE:C	2.55	0.42
1:L:67:SER:C	1:L:69:ILE:N	2.73	0.42
1:M:319:ASN:O	1:M:320:LYS:C	2.58	0.42
1:N:91:LYS:HZ1	1:N:99:GLU:CD	2.21	0.42
1:O:264:VAL:O	1:O:295:TRP:HB3	2.19	0.42
1:P:187:GLU:HG2	1:P:187:GLU:O	2.18	0.42
1:P:281:LEU:O	1:P:282:ASN:C	2.54	0.42
1:P:58:PHE:CE1	1:P:310:LEU:HD13	2.54	0.42
1:A:203:TYR:OH	1:D:2:HIS:HA	2.19	0.42
1:D:354:GLN:HG2	1:D:356:LEU:CD2	2.50	0.42
1:E:79:PHE:O	1:E:80:HIS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ASP:HA	1:F:147:TRP:CZ3	2.53	0.42
1:H:172:ARG:HH22	1:H:176:ILE:HD11	1.81	0.42
1:I:177:CYS:HB3	1:I:182:LEU:HB2	2.01	0.42
1:J:209:LEU:HA	1:J:209:LEU:HD23	1.72	0.42
1:K:22:ILE:O	1:K:22:ILE:CG2	2.66	0.42
1:K:244:THR:CG2	1:K:247:GLN:HG3	2.49	0.42
1:L:91:LYS:HD3	1:L:96:ILE:HG13	2.01	0.42
1:N:250:MET:O	1:N:254:THR:OG1	2.23	0.42
1:O:58:PHE:HE2	1:O:62:LEU:HD11	1.84	0.42
1:P:106:ILE:CG2	1:P:142:VAL:HG11	2.50	0.42
1:P:154:ALA:O	1:P:155:ASP:C	2.57	0.42
1:R:152:ARG:HH11	1:R:152:ARG:HD3	1.56	0.42
1:A:184:PRO:HD2	1:A:225:GLY:O	2.18	0.42
1:A:42:ARG:HD2	1:A:357:PHE:CG	2.53	0.42
1:C:118:THR:CG2	1:C:121:GLU:CB	2.98	0.42
1:C:152:ARG:HD3	1:C:152:ARG:HH11	1.28	0.42
1:A:207:LYS:CE	1:D:2:HIS:NE2	2.69	0.42
1:F:201:CYS:SG	1:F:233:VAL:HG13	2.59	0.42
1:H:86:LYS:HD3	1:H:90:GLY:HA2	2.02	0.42
1:J:75:GLY:HA2	1:J:103:VAL:O	2.20	0.42
1:J:144:PHE:CE1	1:J:185:ILE:HD11	2.54	0.42
1:J:67:SER:O	1:J:69:ILE:N	2.53	0.42
1:K:106:ILE:HD12	1:K:107:LYS:H	1.84	0.42
1:K:330:ARG:HA	1:K:330:ARG:HE	1.84	0.42
1:K:344:HIS:CE1	1:K:346:GLY:HA2	2.54	0.42
1:L:48:VAL:HG12	1:L:54:ASN:HD22	1.85	0.42
1:M:146:LYS:C	1:M:146:LYS:HD3	2.40	0.42
1:N:1:ALA:O	1:N:3:ARG:NH2	2.52	0.42
1:N:267:ILE:HD13	1:N:267:ILE:HG21	1.39	0.42
1:R:213:TYR:OH	1:R:228:LEU:HD13	2.19	0.42
1:A:256:LEU:HD13	1:A:267:ILE:HD11	2.01	0.42
1:A:279:ALA:HB1	1:A:301:TYR:CZ	2.55	0.42
1:B:29:ILE:HG21	1:B:29:ILE:HD13	1.73	0.42
1:F:8:THR:OG1	1:F:11:GLN:HG3	2.19	0.42
1:I:206:GLU:HG2	1:I:255:ALA:HA	2.01	0.42
1:I:313:TRP:HA	1:I:319:ASN:CB	2.50	0.42
1:J:198:LEU:CD1	1:J:234:THR:HA	2.50	0.42
1:I:121:GLU:OE1	1:J:1:ALA:HB2	2.20	0.42
1:J:43:LEU:O	1:J:44:GLN:C	2.53	0.42
1:K:29:ILE:HG21	1:K:29:ILE:HD13	1.76	0.42
1:L:3:ARG:HB2	1:L:4:PHE:H	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:323:THR:O	1:M:324:GLN:C	2.58	0.42
1:O:4:PHE:CZ	1:P:119:ASN:HB2	2.54	0.42
1:P:3:ARG:CD	1:P:4:PHE:H	2.08	0.42
1:Q:44:GLN:OE1	1:Q:44:GLN:HA	2.18	0.42
1:R:119:ASN:O	1:R:152:ARG:NH1	2.36	0.42
1:B:136:GLN:O	1:B:137:TYR:C	2.57	0.42
1:C:4:PHE:CE1	1:D:119:ASN:HB2	2.54	0.42
1:D:214:LYS:HD3	1:D:214:LYS:HA	1.81	0.42
1:F:171:ALA:HA	1:F:216:LEU:CD1	2.49	0.42
1:F:33:ASP:CB	1:F:77:ILE:HG22	2.47	0.42
1:G:271:SER:O	1:G:272:GLY:C	2.57	0.42
1:I:8:THR:OG1	1:I:11:GLN:HG3	2.19	0.42
1:J:208:VAL:O	1:J:212:VAL:HG23	2.20	0.42
1:K:18:ILE:O	1:K:19:ALA:C	2.56	0.42
1:K:349:GLY:H	1:O:86:LYS:NZ	2.17	0.42
1:M:172:ARG:O	1:M:176:ILE:HG13	2.19	0.42
1:N:211:ALA:O	1:N:212:VAL:C	2.58	0.42
1:I:240:THR:HB	1:N:240:THR:HB	2.00	0.42
1:N:259:THR:O	1:N:261:PRO:HD3	2.20	0.42
1:O:128:ASP:HA	1:P:125:GLN:NE2	2.30	0.42
1:Q:121:GLU:OE2	1:Q:158:PRO:HA	2.20	0.42
1:Q:174:ALA:O	1:Q:178:GLN:HG3	2.19	0.42
1:Q:335:CYS:O	1:Q:336:GLN:C	2.58	0.42
1:R:191:ILE:HB	1:R:192:PRO:HD2	2.01	0.42
1:A:67:SER:C	1:A:69:ILE:N	2.72	0.42
1:B:284:ASN:OD1	1:B:340:GLY:HA2	2.20	0.42
1:B:330:ARG:HH21	1:B:333:ALA:CB	2.32	0.42
1:B:48:VAL:HG12	1:B:54:ASN:ND2	2.34	0.42
1:C:147:TRP:HB2	1:C:173:TYR:CE1	2.54	0.42
1:C:171:ALA:HB1	1:C:219:HIS:CG	2.55	0.42
1:E:213:TYR:OH	1:E:228:LEU:HD13	2.20	0.42
1:F:250:MET:CE	1:F:291:LEU:HD21	2.49	0.42
1:H:44:GLN:HA	1:H:44:GLN:OE1	2.20	0.42
1:K:29:ILE:HB	1:K:300:SER:HA	2.00	0.42
1:N:171:ALA:HB1	1:N:219:HIS:CG	2.54	0.42
1:N:216:LEU:HB3	1:N:221:VAL:HB	2.00	0.42
1:O:231:ASN:HA	1:O:270:LEU:HG	2.01	0.42
1:O:287:ASN:O	1:O:293:LYS:NZ	2.53	0.42
1:P:123:THR:HG21	1:P:165:GLU:OE2	2.19	0.42
1:P:130:LEU:O	1:P:131:SER:C	2.56	0.42
1:P:165:GLU:O	1:P:166:ASN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:299:PHE:HB2	1:P:301:TYR:CD2	2.55	0.42
1:Q:165:GLU:HB2	3:Q:2003:HOH:O	2.19	0.42
1:R:244:THR:HG23	1:R:246:GLU:OE1	2.20	0.42
1:A:344:HIS:N	1:A:344:HIS:ND1	2.65	0.42
1:B:1:ALA:N	1:B:220:HIS:HE1	2.18	0.42
1:B:320:LYS:O	1:B:324:GLN:HG3	2.20	0.42
1:D:354:GLN:HB3	1:D:355:SER:H	1.56	0.42
1:E:231:ASN:HA	1:E:270:LEU:HG	2.01	0.42
1:F:248:VAL:O	1:F:249:ALA:C	2.55	0.42
1:L:294:PRO:HD2	1:L:295:TRP:CZ2	2.55	0.42
1:L:320:LYS:O	1:L:324:GLN:HG3	2.20	0.42
1:M:2:HIS:O	1:M:4:PHE:HD1	2.02	0.42
1:N:294:PRO:HD2	1:N:295:TRP:CZ2	2.55	0.42
1:O:105:GLY:HA2	1:O:144:PHE:O	2.20	0.42
1:P:236:GLY:O	1:P:237:HIS:C	2.58	0.42
1:Q:33:ASP:O	1:Q:107:LYS:HE3	2.19	0.42
1:R:118:THR:HG23	1:R:121:GLU:H	1.85	0.42
1:C:94:ARG:O	1:C:98:LYS:HG3	2.20	0.42
1:C:91:LYS:NZ	1:C:99:GLU:OE1	2.47	0.42
1:F:165:GLU:OE1	3:F:402:HOH:O	2.21	0.42
1:F:259:THR:O	1:F:261:PRO:HD3	2.19	0.42
1:H:83:LEU:HG	1:H:83:LEU:O	2.20	0.42
1:I:85:GLN:O	1:I:92:LEU:HD23	2.20	0.42
1:K:156:GLN:O	1:L:1:ALA:HB2	2.20	0.42
1:L:22:ILE:O	1:L:22:ILE:HG22	2.20	0.42
1:L:325:GLU:O	1:L:326:ALA:C	2.58	0.42
1:M:1:ALA:HA	1:N:159:SER:HB3	2.01	0.42
1:N:106:ILE:HA	1:N:106:ILE:HD12	1.82	0.42
1:N:325:GLU:O	1:N:328:MET:HB3	2.19	0.42
1:O:77:ILE:HD13	1:O:77:ILE:HG21	1.74	0.42
1:P:115:LEU:HD12	1:P:115:LEU:HA	1.94	0.42
1:Q:130:LEU:O	1:Q:133:ARG:HB2	2.20	0.42
1:Q:43:LEU:HA	1:Q:43:LEU:HD23	1.86	0.42
1:R:87:ASP:C	1:R:89:GLN:H	2.22	0.42
1:A:118:THR:HG23	1:A:121:GLU:HB2	2.00	0.42
1:A:172:ARG:NH2	1:A:176:ILE:HD11	2.35	0.42
1:E:9:GLN:NE2	1:E:9:GLN:HA	2.35	0.42
1:G:250:MET:CE	1:G:291:LEU:HD22	2.50	0.42
1:G:65:VAL:O	1:G:66:ASP:HB3	2.20	0.42
1:I:109:ASP:C	1:I:109:ASP:OD1	2.59	0.42
1:I:66:ASP:OD1	1:I:67:SER:CA	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:345:THR:HG23	1:J:345:THR:O	2.19	0.42
1:J:44:GLN:O	1:J:47:LYS:N	2.45	0.42
1:K:357:PHE:C	1:O:139:LYS:NZ	2.73	0.42
1:M:4:PHE:CE1	1:N:119:ASN:HB2	2.55	0.42
1:N:249:ALA:HB1	1:N:286:ILE:HA	2.02	0.42
1:N:59:ARG:HB3	1:N:63:PHE:CE1	2.55	0.42
1:P:332:MET:HG2	3:P:552:HOH:O	2.19	0.42
1:P:87:ASP:OD2	1:P:91:LYS:HB3	2.20	0.42
1:Q:87:ASP:HB3	1:Q:89:GLN:H	1.84	0.42
1:R:28:GLY:HA3	1:R:299:PHE:CZ	2.55	0.42
1:B:18:ILE:HB	1:B:183:VAL:HG23	2.02	0.41
1:B:194:GLY:O	1:B:238:ALA:N	2.39	0.41
1:C:240:THR:O	1:C:242:LYS:HE3	2.19	0.41
1:D:84:TYR:OH	1:D:140:ASP:OD2	2.28	0.41
1:E:329:LYS:CE	1:E:346:GLY:O	2.56	0.41
1:F:147:TRP:CD1	1:F:170:LEU:HD23	2.55	0.41
1:H:329:LYS:NZ	1:H:347:SER:O	2.46	0.41
1:I:115:LEU:HD13	1:I:123:THR:OG1	2.20	0.41
1:I:152:ARG:HH11	1:I:152:ARG:HD3	1.33	0.41
1:I:53:GLU:CD	1:I:56:ARG:HE	2.23	0.41
1:K:146:LYS:HE2	1:K:187:GLU:OE1	2.19	0.41
1:L:229:LYS:NZ	1:L:300:SER:OG	2.21	0.41
1:L:33:ASP:OD2	1:L:107:LYS:HB2	2.20	0.41
1:M:117:GLY:O	1:N:3:ARG:CD	2.67	0.41
1:N:324:GLN:O	1:N:328:MET:HB2	2.20	0.41
1:N:3:ARG:H	1:N:3:ARG:CD	2.32	0.41
1:P:216:LEU:HD12	1:P:216:LEU:HA	1.68	0.41
1:R:123:THR:HG22	1:R:124:ILE:H	1.85	0.41
1:R:313:TRP:CE2	1:R:315:GLY:HA2	2.54	0.41
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.73	0.41
1:A:4:PHE:CE1	1:B:119:ASN:HB2	2.55	0.41
1:B:133:ARG:O	1:B:134:CYS:C	2.58	0.41
1:B:280:THR:O	1:B:281:LEU:C	2.59	0.41
1:B:28:GLY:HA3	1:B:299:PHE:CE2	2.55	0.41
1:B:42:ARG:HD2	1:B:42:ARG:HH11	1.54	0.41
1:C:267:ILE:HD13	1:C:267:ILE:HG21	1.47	0.41
1:G:15:LEU:HA	1:G:15:LEU:HD23	1.85	0.41
1:H:276:GLU:HG3	1:H:352:SER:HB3	2.03	0.41
1:I:72:SER:HB3	1:I:331:ALA:O	2.20	0.41
1:J:69:ILE:HG13	1:J:69:ILE:O	2.21	0.41
1:K:227:LEU:HD23	1:K:227:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:294:PRO:HD2	1:O:295:TRP:CZ2	2.55	0.41
1:R:244:THR:N	1:R:247:GLN:OE1	2.53	0.41
1:Q:156:GLN:HE22	1:R:3:ARG:HE	1.40	0.41
1:B:186:VAL:O	1:B:186:VAL:HG12	2.20	0.41
1:D:158:PRO:HG3	1:D:204:VAL:HG13	2.03	0.41
1:E:54:ASN:O	1:E:55:ARG:C	2.58	0.41
1:G:3:ARG:CG	1:H:156:GLN:HE22	2.32	0.41
1:H:187:GLU:HG3	1:H:229:LYS:O	2.21	0.41
1:I:118:THR:HG22	1:I:121:GLU:H	1.78	0.41
1:J:107:LYS:HB2	1:J:107:LYS:HE2	1.79	0.41
1:I:156:GLN:CB	1:J:1:ALA:HB1	2.47	0.41
1:K:244:THR:CG2	1:K:246:GLU:HB2	2.50	0.41
1:M:84:TYR:OH	1:M:140:ASP:OD2	2.24	0.41
1:M:191:ILE:HA	1:M:192:PRO:HD3	1.84	0.41
1:N:66:ASP:OD1	1:N:67:SER:N	2.54	0.41
1:O:335:CYS:O	1:O:339:LYS:HD2	2.20	0.41
1:Q:224:GLU:HB3	3:Q:2026:HOH:O	2.19	0.41
1:A:3:ARG:NH2	1:B:156:GLN:NE2	2.69	0.41
1:B:168:ASN:O	1:B:169:ALA:C	2.59	0.41
1:B:207:LYS:HD3	1:C:2:HIS:CE1	2.56	0.41
1:C:102:ILE:HG21	1:C:102:ILE:HD13	1.82	0.41
1:C:148:ARG:HH21	1:C:148:ARG:HD3	1.67	0.41
1:C:211:ALA:O	1:C:212:VAL:C	2.58	0.41
1:D:182:LEU:HA	1:D:182:LEU:HD23	1.82	0.41
1:F:144:PHE:HB2	1:F:183:VAL:O	2.21	0.41
1:I:319:ASN:N	1:I:319:ASN:OD1	2.52	0.41
1:I:66:ASP:OD1	1:I:67:SER:N	2.53	0.41
1:K:9:GLN:O	1:K:10:GLU:C	2.57	0.41
1:I:2:HIS:NE2	1:L:200:HIS:CE1	2.89	0.41
1:L:3:ARG:NH1	1:L:3:ARG:HG2	2.35	0.41
1:N:78:LEU:HD23	1:N:78:LEU:HA	1.89	0.41
1:P:316:LYS:NZ	3:P:508:HOH:O	2.52	0.41
1:P:43:LEU:O	1:P:44:GLN:C	2.57	0.41
1:Q:18:ILE:HG21	1:Q:18:ILE:HD13	1.79	0.41
1:Q:244:THR:O	1:Q:244:THR:CG2	2.68	0.41
1:R:3:ARG:HB2	1:R:4:PHE:H	1.68	0.41
1:A:42:ARG:O	1:A:45:ARG:HB2	2.21	0.41
1:C:108:LEU:O	1:C:109:ASP:C	2.59	0.41
1:C:172:ARG:HA	1:C:172:ARG:HD2	1.81	0.41
1:C:244:THR:HG23	1:C:244:THR:O	2.17	0.41
1:D:343:VAL:O	1:D:344:HIS:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ILE:HG22	1:E:297:LEU:HD13	2.03	0.41
1:E:67:SER:C	1:E:69:ILE:N	2.69	0.41
1:F:123:THR:HG21	1:F:165:GLU:HG3	2.02	0.41
1:F:354:GLN:HG2	1:F:355:SER:O	2.21	0.41
1:F:46:ILE:O	1:F:47:LYS:C	2.58	0.41
1:H:228:LEU:HG	1:H:230:PRO:HD3	2.02	0.41
1:I:119:ASN:HB2	1:J:4:PHE:CE1	2.56	0.41
1:I:244:THR:O	1:I:245:PRO:C	2.59	0.41
1:I:36:VAL:O	1:I:36:VAL:CG1	2.64	0.41
1:I:4:PHE:CE1	1:J:119:ASN:HB2	2.55	0.41
1:J:93:PHE:HA	1:J:96:ILE:HD12	2.03	0.41
1:K:106:ILE:HG23	1:K:108:LEU:HG	2.01	0.41
1:K:191:ILE:HG23	1:K:191:ILE:HD12	1.80	0.41
1:K:51:THR:HG22	1:K:54:ASN:CB	2.50	0.41
1:M:105:GLY:HA2	1:M:144:PHE:O	2.21	0.41
1:N:63:PHE:O	1:N:100:LYS:NZ	2.53	0.41
1:P:231:ASN:ND2	3:P:505:HOH:O	2.53	0.41
1:R:70:ASN:HD22	1:R:70:ASN:HA	1.38	0.41
1:B:312:ALA:HB1	1:B:322:ALA:HB1	2.02	0.41
1:C:61:ILE:CG2	1:C:324:GLN:HG2	2.50	0.41
1:C:324:GLN:O	1:C:328:MET:HB2	2.21	0.41
1:D:121:GLU:CG	1:D:157:CYS:SG	3.08	0.41
1:E:36:VAL:HG13	1:E:55:ARG:NH1	2.36	0.41
1:H:158:PRO:O	1:H:158:PRO:CG	2.69	0.41
1:H:123:THR:CG2	1:H:165:GLU:HG3	2.50	0.41
1:I:184:PRO:HD2	1:I:225:GLY:O	2.20	0.41
1:K:106:ILE:HD12	1:K:106:ILE:HA	1.74	0.41
1:K:187:GLU:HB2	1:K:229:LYS:HB3	2.01	0.41
1:K:249:ALA:HB1	1:K:286:ILE:HA	2.02	0.41
1:L:267:ILE:HG21	1:L:267:ILE:HD12	1.82	0.41
1:N:306:GLN:O	1:N:309:ALA:HB3	2.20	0.41
1:O:294:PRO:HD2	1:O:295:TRP:CE2	2.54	0.41
1:P:121:GLU:OE2	1:P:158:PRO:HA	2.21	0.41
1:P:276:GLU:HB2	1:P:352:SER:CB	2.46	0.41
1:Q:123:THR:CG2	1:Q:165:GLU:HG3	2.51	0.41
1:Q:129:GLY:N	1:R:125:GLN:HE22	1.96	0.41
1:R:208:VAL:O	1:R:212:VAL:HG23	2.21	0.41
1:A:144:PHE:HB2	1:A:183:VAL:O	2.21	0.41
1:A:280:THR:HG22	1:A:342:TYR:CD2	2.55	0.41
1:C:189:GLU:CD	1:C:191:ILE:HD11	2.41	0.41
1:D:106:ILE:HG23	1:D:108:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ALA:CB	1:D:119:ASN:H	2.33	0.41
1:D:215:ALA:O	1:D:216:LEU:C	2.57	0.41
1:D:230:PRO:O	1:D:270:LEU:HG	2.20	0.41
1:D:335:CYS:O	1:D:338:ALA:HB3	2.21	0.41
1:D:49:GLU:O	1:D:51:THR:N	2.52	0.41
1:F:86:LYS:HG3	1:F:92:LEU:HD23	2.02	0.41
1:I:67:SER:HB3	1:I:68:SER:H	0.83	0.41
1:I:65:VAL:HG12	1:I:69:ILE:HG21	2.02	0.41
1:J:146:LYS:CD	1:J:146:LYS:C	2.89	0.41
1:J:20:GLN:HG2	3:J:563:HOH:O	2.20	0.41
1:L:56:ARG:HG2	1:L:56:ARG:O	2.20	0.41
1:O:172:ARG:HH11	1:O:172:ARG:HD2	1.68	0.41
1:P:191:ILE:HG22	1:P:193:ASP:HB2	2.02	0.41
1:P:227:LEU:HD23	1:P:227:LEU:HA	1.96	0.41
1:P:51:THR:HG23	1:P:53:GLU:N	2.35	0.41
1:Q:144:PHE:HB2	1:Q:183:VAL:O	2.20	0.41
1:Q:77:ILE:HG21	1:Q:77:ILE:HD13	1.66	0.41
1:A:129:GLY:H	1:B:125:GLN:HE22	1.68	0.41
1:C:123:THR:HG23	1:C:165:GLU:HG3	2.01	0.41
1:C:12:LYS:HG2	1:C:222:TYR:CD1	2.56	0.41
3:B:408:HOH:O	1:C:258:ARG:HD2	2.20	0.41
1:B:207:LYS:CD	1:C:2:HIS:NE2	2.80	0.41
1:D:12:LYS:O	1:D:13:LYS:C	2.58	0.41
1:E:306:GLN:O	1:E:307:ALA:C	2.59	0.41
1:E:36:VAL:HG22	1:E:55:ARG:NH2	2.36	0.41
1:I:43:LEU:O	1:I:44:GLN:C	2.58	0.41
1:I:8:THR:HG23	1:I:11:GLN:OE1	2.21	0.41
1:J:223:LEU:O	1:J:226:THR:CG2	2.68	0.41
1:J:342:TYR:OH	1:J:345:THR:CA	2.69	0.41
1:L:244:THR:HG23	1:L:246:GLU:N	2.36	0.41
1:M:106:ILE:CG2	1:M:106:ILE:O	2.68	0.41
1:N:183:VAL:HG12	1:N:183:VAL:O	2.18	0.41
1:O:24:ALA:O	1:O:25:ASN:CB	2.60	0.41
1:O:97:LEU:O	1:O:98:LYS:C	2.58	0.41
1:A:191:ILE:HD13	1:A:191:ILE:HG23	1.78	0.41
1:B:26:GLY:HA3	1:B:339:LYS:HD2	2.03	0.41
1:B:39:MET:HG3	1:B:39:MET:O	2.20	0.41
1:C:143:ASP:O	1:C:182:LEU:HA	2.21	0.41
1:C:75:GLY:HA2	1:C:103:VAL:O	2.20	0.41
1:E:155:ASP:C	1:E:155:ASP:OD1	2.58	0.41
1:F:43:LEU:CD1	1:F:50:ASN:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:PHE:CE2	1:G:310:LEU:HD13	2.56	0.41
1:H:193:ASP:OD1	1:H:193:ASP:N	2.54	0.41
1:H:87:ASP:OD1	1:H:96:ILE:HD11	2.20	0.41
1:J:223:LEU:HA	1:J:223:LEU:HD23	1.88	0.41
1:J:228:LEU:HD23	1:J:267:ILE:HD12	2.02	0.41
1:K:154:ALA:HB3	1:K:157:CYS:HB2	2.03	0.41
1:K:217:ASN:O	1:K:218:ASP:C	2.59	0.41
1:K:50:ASN:HD21	1:K:55:ARG:HD3	1.85	0.41
1:L:121:GLU:OE2	1:L:158:PRO:HA	2.20	0.41
1:L:276:GLU:HG2	1:L:304:ALA:O	2.21	0.41
1:M:244:THR:HG23	1:M:247:GLN:CD	2.41	0.41
1:M:244:THR:CG2	1:M:247:GLN:HG3	2.47	0.41
1:M:125:GLN:NE2	1:N:129:GLY:H	2.19	0.41
1:O:119:ASN:HB3	1:O:157:CYS:SG	2.61	0.41
1:N:203:TYR:OH	1:O:2:HIS:HA	2.20	0.41
1:Q:244:THR:HG22	1:Q:247:GLN:HB2	2.02	0.41
1:Q:73:ILE:HD13	1:Q:73:ILE:HA	1.89	0.41
1:R:129:GLY:O	1:R:130:LEU:C	2.58	0.41
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.51	0.41
1:B:324:GLN:O	1:B:328:MET:HB2	2.21	0.41
1:C:1:ALA:HB3	1:D:119:ASN:N	2.36	0.41
1:C:244:THR:CG2	1:C:247:GLN:CG	2.82	0.41
1:C:249:ALA:HB1	1:C:286:ILE:HA	2.03	0.41
1:E:275:SER:O	1:E:276:GLU:C	2.58	0.41
1:F:270:LEU:C	1:F:270:LEU:HD12	2.41	0.41
1:F:271:SER:CA	1:F:274:MET:HE2	2.51	0.41
1:G:91:LYS:NZ	1:G:99:GLU:OE1	2.52	0.41
1:H:233:VAL:O	1:H:248:VAL:HG13	2.21	0.41
1:H:354:GLN:HG2	1:H:356:LEU:HD23	1.98	0.41
1:H:237:HIS:NE2	1:H:357:PHE:CD2	2.89	0.41
1:H:86:LYS:CG	1:H:90:GLY:HA2	2.50	0.41
1:I:155:ASP:O	1:I:156:GLN:HB2	2.21	0.41
1:J:171:ALA:HA	1:J:216:LEU:HD12	2.02	0.41
1:K:276:GLU:HB3	1:K:330:ARG:HD3	2.03	0.41
1:L:104:VAL:O	1:L:142:VAL:HG13	2.21	0.41
1:L:256:LEU:HD13	1:L:267:ILE:CD1	2.51	0.41
1:M:150:VAL:HG13	1:M:191:ILE:CG1	2.51	0.41
1:M:174:ALA:O	1:M:178:GLN:HG3	2.21	0.41
1:M:81:GLU:O	1:M:85:GLN:HG3	2.21	0.41
1:P:153:ILE:HG12	1:P:204:VAL:HG21	2.02	0.41
1:P:51:THR:HG23	1:P:53:GLU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:276:GLU:OE1	1:R:330:ARG:HD2	2.21	0.41
1:A:12:LYS:HG2	1:A:222:TYR:CE1	2.56	0.41
1:A:274:MET:HA	3:A:509:HOH:O	2.20	0.41
1:C:156:GLN:HE22	1:D:3:ARG:CD	2.31	0.41
1:C:22:ILE:HD13	1:C:22:ILE:HG21	1.91	0.41
1:C:244:THR:O	1:C:247:GLN:N	2.47	0.41
1:C:28:GLY:O	1:C:74:GLY:N	2.50	0.41
1:C:313:TRP:HA	1:C:323:THR:OG1	2.20	0.41
1:C:313:TRP:CH2	1:C:315:GLY:HA2	2.52	0.41
1:C:61:ILE:HG23	1:C:324:GLN:CG	2.51	0.41
1:D:244:THR:HG23	1:D:246:GLU:N	2.29	0.41
1:E:118:THR:HG23	1:E:121:GLU:H	1.84	0.41
1:G:18:ILE:HG21	1:G:18:ILE:HD13	1.83	0.41
1:G:311:ALA:O	1:G:312:ALA:C	2.58	0.41
1:H:152:ARG:HD3	1:H:152:ARG:HH11	1.49	0.41
1:H:12:LYS:HG2	1:H:222:TYR:CE1	2.56	0.41
1:I:28:GLY:HA3	1:I:299:PHE:CE1	2.56	0.41
1:J:142:VAL:HG12	1:J:143:ASP:N	2.36	0.41
1:I:156:GLN:HE22	1:J:3:ARG:CG	2.32	0.41
1:L:164:GLN:HG2	1:L:165:GLU:N	2.36	0.41
1:M:224:GLU:OE2	1:P:258:ARG:NH1	2.44	0.41
1:M:223:LEU:O	1:M:226:THR:HB	2.21	0.41
1:M:4:PHE:O	1:N:117:GLY:HA2	2.21	0.41
1:N:106:ILE:O	1:N:106:ILE:HG23	2.21	0.41
1:N:339:LYS:O	1:N:341:GLN:HG3	2.20	0.41
1:N:68:SER:C	1:N:70:ASN:N	2.73	0.41
1:P:281:LEU:H	1:P:281:LEU:HG	1.69	0.41
1:A:3:ARG:HD2	1:A:3:ARG:N	2.32	0.40
1:A:94:ARG:HD2	1:A:140:ASP:O	2.20	0.40
1:C:78:LEU:O	1:C:106:ILE:HD12	2.21	0.40
1:C:198:LEU:HD22	1:C:243:TYR:CD2	2.56	0.40
1:F:244:THR:HA	1:F:245:PRO:HD3	1.98	0.40
1:G:313:TRP:CD2	1:G:315:GLY:CA	3.04	0.40
1:G:313:TRP:CE2	1:G:315:GLY:CA	3.01	0.40
1:H:273:GLY:CA	1:H:357:PHE:HA	2.51	0.40
1:H:89:GLN:HE21	1:H:89:GLN:HB2	1.70	0.40
1:I:124:ILE:HG21	1:I:147:TRP:CE2	2.55	0.40
1:I:66:ASP:O	1:I:69:ILE:HG22	2.20	0.40
1:J:349:GLY:O	1:J:351:ALA:N	2.53	0.40
1:O:138:LYS:HD2	3:O:505:HOH:O	2.20	0.40
1:P:264:VAL:HA	1:P:265:PRO:HD2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:290:PRO:C	1:P:291:LEU:HG	2.35	0.40
1:P:67:SER:C	1:P:69:ILE:N	2.75	0.40
1:R:2:HIS:O	1:R:4:PHE:HD1	2.03	0.40
1:C:128:ASP:OD2	1:D:128:ASP:HB2	2.21	0.40
1:D:216:LEU:HD12	1:D:216:LEU:HA	1.66	0.40
1:D:249:ALA:HB2	1:D:285:ALA:HB3	2.02	0.40
1:E:18:ILE:HD13	1:E:143:ASP:HB3	2.03	0.40
1:F:50:ASN:ND2	1:F:50:ASN:C	2.74	0.40
1:I:294:PRO:HD2	1:I:295:TRP:CE2	2.55	0.40
1:J:184:PRO:HD2	1:J:225:GLY:O	2.22	0.40
1:K:58:PHE:CE2	1:K:310:LEU:HD13	2.55	0.40
1:M:244:THR:O	1:M:245:PRO:C	2.60	0.40
1:N:36:VAL:HG13	1:N:55:ARG:CZ	2.51	0.40
1:O:78:LEU:O	1:O:106:ILE:HA	2.21	0.40
1:P:343:VAL:O	1:P:344:HIS:HB3	2.20	0.40
1:Q:156:GLN:HB3	1:R:1:ALA:HA	2.01	0.40
1:Q:191:ILE:HG22	1:Q:193:ASP:HB2	2.02	0.40
1:R:171:ALA:O	1:R:172:ARG:C	2.60	0.40
1:R:86:LYS:HD3	1:R:90:GLY:HA2	2.03	0.40
1:A:116:ALA:HB3	3:A:507:HOH:O	2.20	0.40
1:B:51:THR:HG22	1:B:54:ASN:CA	2.49	0.40
1:F:118:THR:CG2	1:F:121:GLU:H	2.35	0.40
1:G:244:THR:HG22	1:G:247:GLN:CG	2.51	0.40
1:G:260:VAL:HA	1:G:261:PRO:HD3	1.86	0.40
1:H:276:GLU:H	1:H:352:SER:HG	1.68	0.40
1:H:98:LYS:O	1:H:99:GLU:C	2.57	0.40
1:I:240:THR:O	1:I:242:LYS:HE3	2.22	0.40
1:K:226:THR:HG23	3:K:512:HOH:O	2.08	0.40
1:K:271:SER:O	1:K:274:MET:HE2	2.21	0.40
1:L:196:HIS:O	1:L:239:CYS:HB2	2.21	0.40
1:O:73:ILE:HA	1:O:73:ILE:HD13	1.86	0.40
1:P:198:LEU:HD22	1:P:243:TYR:CD2	2.56	0.40
1:Q:189:GLU:HB2	1:Q:270:LEU:CD2	2.51	0.40
1:R:299:PHE:HB2	1:R:301:TYR:CD1	2.56	0.40
1:B:12:LYS:O	1:B:13:LYS:C	2.60	0.40
1:C:155:ASP:OD1	1:C:156:GLN:HG3	2.21	0.40
1:B:203:TYR:OH	1:C:2:HIS:ND1	2.27	0.40
1:F:227:LEU:HA	1:F:227:LEU:HD23	1.84	0.40
1:F:344:HIS:CD2	1:F:345:THR:N	2.89	0.40
1:G:161:LEU:HD11	1:H:219:HIS:CE1	2.56	0.40
1:H:25:ASN:H	1:H:27:LYS:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:GLU:HG2	1:H:304:ALA:O	2.21	0.40
1:I:1:ALA:HB2	1:J:159:SER:HB3	2.03	0.40
1:J:354:GLN:HG2	1:J:354:GLN:O	2.20	0.40
1:K:120:LYS:CB	1:K:152:ARG:HH12	2.33	0.40
1:L:118:THR:CG2	1:L:121:GLU:CB	2.99	0.40
1:L:118:THR:HG21	1:L:121:GLU:CB	2.51	0.40
1:L:136:GLN:HE21	1:L:136:GLN:HB2	1.61	0.40
1:M:189:GLU:CD	1:M:191:ILE:CD1	2.90	0.40
1:M:18:ILE:HG21	1:M:18:ILE:HD13	1.79	0.40
1:M:21:SER:OG	1:M:22:ILE:N	2.55	0.40
1:N:187:GLU:HG3	1:N:229:LYS:O	2.21	0.40
1:N:231:ASN:HA	1:N:270:LEU:HG	2.02	0.40
1:O:271:SER:CA	1:O:274:MET:HE2	2.52	0.40
1:O:4:PHE:CD1	1:P:119:ASN:HB2	2.56	0.40
1:P:133:ARG:O	1:P:137:TYR:CD2	2.75	0.40
1:A:229:LYS:HA	1:A:268:CYS:O	2.21	0.40
1:B:28:GLY:CA	1:B:299:PHE:CZ	3.05	0.40
1:B:58:PHE:HE2	1:B:62:LEU:HD11	1.85	0.40
1:E:12:LYS:HE2	1:E:222:TYR:CD1	2.56	0.40
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.69	0.40
1:F:271:SER:O	1:F:272:GLY:C	2.59	0.40
1:G:330:ARG:NE	1:G:330:ARG:HA	2.34	0.40
1:I:49:GLU:O	1:I:51:THR:N	2.54	0.40
1:I:66:ASP:OD1	1:I:67:SER:CB	2.70	0.40
1:J:267:ILE:HG21	1:J:267:ILE:HD13	1.85	0.40
1:K:63:PHE:N	1:K:63:PHE:CD2	2.87	0.40
1:O:163:ILE:HD13	1:O:163:ILE:HG21	1.87	0.40
1:Q:118:THR:HG23	1:Q:119:ASN:N	2.35	0.40
1:R:131:SER:O	1:R:132:GLU:C	2.60	0.40
1:R:147:TRP:HB3	1:R:173:TYR:CE2	2.56	0.40
1:R:89:GLN:O	1:R:89:GLN:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/363 (99%)	324 (90%)	27 (8%)	7 (2%)	9	14
1	B	346/363 (95%)	300 (87%)	35 (10%)	11 (3%)	5	6
1	C	343/363 (94%)	317 (92%)	22 (6%)	4 (1%)	15	27
1	D	354/363 (98%)	319 (90%)	24 (7%)	11 (3%)	5	6
1	E	352/363 (97%)	316 (90%)	25 (7%)	11 (3%)	5	6
1	F	351/363 (97%)	315 (90%)	25 (7%)	11 (3%)	5	6
1	G	342/363 (94%)	311 (91%)	25 (7%)	6 (2%)	10	17
1	H	355/363 (98%)	319 (90%)	22 (6%)	14 (4%)	3	4
1	I	342/363 (94%)	300 (88%)	34 (10%)	8 (2%)	7	11
1	J	354/363 (98%)	320 (90%)	24 (7%)	10 (3%)	6	8
1	K	352/363 (97%)	325 (92%)	22 (6%)	5 (1%)	13	23
1	L	342/363 (94%)	307 (90%)	30 (9%)	5 (2%)	12	21
1	M	358/363 (99%)	318 (89%)	29 (8%)	11 (3%)	5	6
1	N	342/363 (94%)	307 (90%)	29 (8%)	6 (2%)	10	17
1	O	342/363 (94%)	305 (89%)	33 (10%)	4 (1%)	15	27
1	P	358/363 (99%)	328 (92%)	23 (6%)	7 (2%)	9	14
1	Q	342/363 (94%)	319 (93%)	18 (5%)	5 (2%)	12	21
1	R	342/363 (94%)	316 (92%)	23 (7%)	3 (1%)	20	36
All	All	6275/6534 (96%)	5666 (90%)	470 (8%)	139 (2%)	8	12

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	3	ARG
1	A	87	ASP
1	A	357	PHE
1	B	69	ILE
1	B	342	TYR
1	B	345	THR
1	C	272	GLY
1	D	89	GLN
1	D	90	GLY
1	D	354	GLN

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Mol	Chain	Res	Type
1	E	2	HIS
1	E	89	GLN
1	E	196	HIS
1	E	345	THR
1	E	350	ALA
1	E	352	SER
1	F	345	THR
1	F	352	SER
1	F	353	THR
1	F	355	SER
1	H	3	ARG
1	H	89	GLN
1	H	90	GLY
1	H	344	HIS
1	H	345	THR
1	H	346	GLY
1	H	347	SER
1	H	350	ALA
1	H	354	GLN
1	I	3	ARG
1	I	67	SER
1	I	69	ILE
1	I	272	GLY
1	J	3	ARG
1	J	196	HIS
1	J	345	THR
1	J	351	ALA
1	K	346	GLY
1	L	3	ARG
1	L	272	GLY
1	M	3	ARG
1	M	67	SER
1	M	68	SER
1	M	70	ASN
1	M	344	HIS
1	M	353	THR
1	O	2	HIS
1	O	272	GLY
1	O	343	VAL
1	P	2	HIS
1	P	3	ARG
1	Q	87	ASP

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Mol	Chain	Res	Type
1	R	3	ARG
1	A	154	ALA
1	A	344	HIS
1	B	68	SER
1	B	70	ASN
1	B	90	GLY
1	B	272	GLY
1	B	346	GLY
1	B	347	SER
1	C	3	ARG
1	C	87	ASP
1	C	344	HIS
1	D	70	ASN
1	D	87	ASP
1	D	346	GLY
1	D	347	SER
1	D	355	SER
1	E	67	SER
1	E	347	SER
1	F	70	ASN
1	F	272	GLY
1	G	2	HIS
1	G	65	VAL
1	G	67	SER
1	G	70	ASN
1	G	272	GLY
1	H	2	HIS
1	H	67	SER
1	H	272	GLY
1	H	355	SER
1	J	68	SER
1	J	272	GLY
1	J	347	SER
1	J	348	SER
1	K	89	GLN
1	K	348	SER
1	M	272	GLY
1	M	352	SER
1	N	3	ARG
1	N	65	VAL
1	N	69	ILE
1	N	87	ASP

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Mol	Chain	Res	Type
1	N	272	GLY
1	O	320	LYS
1	Q	3	ARG
1	Q	272	GLY
1	R	272	GLY
1	B	67	SER
1	B	89	GLN
1	D	3	ARG
1	F	351	ALA
1	G	66	ASP
1	K	347	SER
1	M	345	THR
1	M	355	SER
1	P	355	SER
1	Q	2	HIS
1	D	344	HIS
1	F	350	ALA
1	I	80	HIS
1	I	224	GLU
1	P	87	ASP
1	P	230	PRO
1	R	196	HIS
1	D	188	PRO
1	E	164	GLN
1	F	274	MET
1	H	196	HIS
1	J	355	SER
1	L	70	ASN
1	N	4	PHE
1	F	188	PRO
1	L	320	LYS
1	F	191	ILE
1	A	230	PRO
1	E	188	PRO
1	I	4	PHE
1	I	343	VAL
1	L	46	ILE
1	Q	188	PRO
1	E	163	ILE
1	K	230	PRO
1	P	188	PRO
1	J	343	VAL

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Mol	Chain	Res	Type
1	P	272	GLY
1	M	314	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/290 (99%)	250 (87%)	37 (13%)	5	9
1	B	279/290 (96%)	244 (88%)	35 (12%)	5	10
1	C	277/290 (96%)	240 (87%)	37 (13%)	4	8
1	D	284/290 (98%)	250 (88%)	34 (12%)	6	11
1	E	282/290 (97%)	247 (88%)	35 (12%)	5	10
1	F	282/290 (97%)	241 (86%)	41 (14%)	4	7
1	G	276/290 (95%)	238 (86%)	38 (14%)	4	8
1	H	285/290 (98%)	252 (88%)	33 (12%)	6	12
1	I	276/290 (95%)	236 (86%)	40 (14%)	4	7
1	J	284/290 (98%)	249 (88%)	35 (12%)	5	10
1	K	283/290 (98%)	249 (88%)	34 (12%)	6	11
1	L	276/290 (95%)	240 (87%)	36 (13%)	5	9
1	M	287/290 (99%)	256 (89%)	31 (11%)	7	14
1	N	276/290 (95%)	242 (88%)	34 (12%)	5	10
1	O	276/290 (95%)	243 (88%)	33 (12%)	6	11
1	P	287/290 (99%)	255 (89%)	32 (11%)	7	13
1	Q	276/290 (95%)	245 (89%)	31 (11%)	7	13
1	R	276/290 (95%)	244 (88%)	32 (12%)	6	12
All	All	5049/5220 (97%)	4421 (88%)	628 (12%)	5	10

All (628) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	3	ARG
1	A	10	GLU
1	A	25	ASN
1	A	45	ARG
1	A	51	THR
1	A	69	ILE
1	A	81	GLU
1	A	87	ASP
1	A	89	GLN
1	A	100	LYS
1	A	106	ILE
1	A	109	ASP
1	A	115	LEU
1	A	118	THR
1	A	123	THR
1	A	131	SER
1	A	146	LYS
1	A	152	ARG
1	A	160	SER
1	A	191	ILE
1	A	199	GLU
1	A	200	HIS
1	A	216	LEU
1	A	226	THR
1	A	230	PRO
1	A	237	HIS
1	A	244	THR
1	A	258	ARG
1	A	267	ILE
1	A	291	LEU
1	A	295	TRP
1	A	310	LEU
1	A	328	MET
1	A	330	ARG
1	A	348	SER
1	A	355	SER
1	B	3	ARG
1	B	7	LEU
1	B	9	GLN
1	B	10	GLU
1	B	25	ASN
1	B	27	LYS

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Mol	Chain	Res	Type
1	B	45	ARG
1	B	51	THR
1	B	67	SER
1	B	71	GLN
1	B	94	ARG
1	B	118	THR
1	B	123	THR
1	B	124	ILE
1	B	164	GLN
1	B	173	TYR
1	B	183	VAL
1	B	199	GLU
1	B	200	HIS
1	B	226	THR
1	B	227	LEU
1	B	230	PRO
1	B	244	THR
1	B	258	ARG
1	B	267	ILE
1	B	291	LEU
1	B	295	TRP
1	B	296	LYS
1	B	303	ARG
1	B	310	LEU
1	B	325	GLU
1	B	330	ARG
1	B	339	LYS
1	B	344	HIS
1	B	345	THR
1	C	2	HIS
1	C	3	ARG
1	C	9	GLN
1	C	10	GLU
1	C	16	SER
1	C	44	GLN
1	C	50	ASN
1	C	51	THR
1	C	53	GLU
1	C	89	GLN
1	C	94	ARG
1	C	110	GLN
1	C	115	LEU

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Mol	Chain	Res	Type
1	C	118	THR
1	C	123	THR
1	C	131	SER
1	C	146	LYS
1	C	151	LEU
1	C	152	ARG
1	C	157	CYS
1	C	160	SER
1	C	164	GLN
1	C	191	ILE
1	C	195	ASP
1	C	199	GLU
1	C	200	HIS
1	C	207	LYS
1	C	216	LEU
1	C	226	THR
1	C	231	ASN
1	C	237	HIS
1	C	257	HIS
1	C	274	MET
1	C	291	LEU
1	C	295	TRP
1	C	303	ARG
1	C	325	GLU
1	D	30	LEU
1	D	44	GLN
1	D	50	ASN
1	D	51	THR
1	D	65	VAL
1	D	68	SER
1	D	70	ASN
1	D	81	GLU
1	D	87	ASP
1	D	109	ASP
1	D	118	THR
1	D	123	THR
1	D	146	LYS
1	D	193	ASP
1	D	199	GLU
1	D	200	HIS
1	D	207	LYS
1	D	214	LYS

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Mol	Chain	Res	Type
1	D	216	LEU
1	D	217	ASN
1	D	226	THR
1	D	231	ASN
1	D	244	THR
1	D	250	MET
1	D	257	HIS
1	D	258	ARG
1	D	291	LEU
1	D	295	TRP
1	D	303	ARG
1	D	310	LEU
1	D	328	MET
1	D	347	SER
1	D	348	SER
1	D	355	SER
1	E	2	HIS
1	E	3	ARG
1	E	10	GLU
1	E	45	ARG
1	E	51	THR
1	E	67	SER
1	E	69	ILE
1	E	72	SER
1	E	115	LEU
1	E	118	THR
1	E	123	THR
1	E	131	SER
1	E	132	GLU
1	E	148	ARG
1	E	152	ARG
1	E	160	SER
1	E	173	TYR
1	E	193	ASP
1	E	200	HIS
1	E	216	LEU
1	E	226	THR
1	E	230	PRO
1	E	237	HIS
1	E	244	THR
1	E	257	HIS
1	E	267	ILE

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Mol	Chain	Res	Type
1	E	293	LYS
1	E	295	TRP
1	E	303	ARG
1	E	310	LEU
1	E	325	GLU
1	E	328	MET
1	E	345	THR
1	E	348	SER
1	E	352	SER
1	F	16	SER
1	F	45	ARG
1	F	50	ASN
1	F	51	THR
1	F	68	SER
1	F	69	ILE
1	F	71	GLN
1	F	89	GLN
1	F	94	ARG
1	F	98	LYS
1	F	100	LYS
1	F	110	GLN
1	F	115	LEU
1	F	118	THR
1	F	123	THR
1	F	124	ILE
1	F	131	SER
1	F	151	LEU
1	F	152	ARG
1	F	164	GLN
1	F	173	TYR
1	F	191	ILE
1	F	216	LEU
1	F	217	ASN
1	F	226	THR
1	F	231	ASN
1	F	245	PRO
1	F	250	MET
1	F	258	ARG
1	F	267	ILE
1	F	274	MET
1	F	291	LEU
1	F	295	TRP

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Mol	Chain	Res	Type
1	F	310	LEU
1	F	325	GLU
1	F	328	MET
1	F	329	LYS
1	F	330	ARG
1	F	345	THR
1	F	352	SER
1	F	353	THR
1	G	16	SER
1	G	45	ARG
1	G	51	THR
1	G	70	ASN
1	G	72	SER
1	G	87	ASP
1	G	89	GLN
1	G	98	LYS
1	G	109	ASP
1	G	115	LEU
1	G	118	THR
1	G	123	THR
1	G	131	SER
1	G	158	PRO
1	G	164	GLN
1	G	173	TYR
1	G	195	ASP
1	G	198	LEU
1	G	199	GLU
1	G	200	HIS
1	G	207	LYS
1	G	214	LYS
1	G	216	LEU
1	G	217	ASN
1	G	224	GLU
1	G	226	THR
1	G	231	ASN
1	G	232	MET
1	G	244	THR
1	G	250	MET
1	G	257	HIS
1	G	267	ILE
1	G	274	MET
1	G	291	LEU

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Mol	Chain	Res	Type
1	G	295	TRP
1	G	303	ARG
1	G	310	LEU
1	G	330	ARG
1	H	3	ARG
1	H	9	GLN
1	H	10	GLU
1	H	45	ARG
1	H	50	ASN
1	H	51	THR
1	H	67	SER
1	H	70	ASN
1	H	81	GLU
1	H	109	ASP
1	H	118	THR
1	H	123	THR
1	H	131	SER
1	H	132	GLU
1	H	139	LYS
1	H	151	LEU
1	H	152	ARG
1	H	158	PRO
1	H	160	SER
1	H	164	GLN
1	H	195	ASP
1	H	199	GLU
1	H	216	LEU
1	H	226	THR
1	H	239	CYS
1	H	244	THR
1	H	257	HIS
1	H	267	ILE
1	H	295	TRP
1	H	296	LYS
1	H	310	LEU
1	H	329	LYS
1	H	352	SER
1	I	3	ARG
1	I	10	GLU
1	I	16	SER
1	I	34	GLU
1	I	42	ARG

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Mol	Chain	Res	Type
1	I	44	GLN
1	I	45	ARG
1	I	57	GLN
1	I	59	ARG
1	I	65	VAL
1	I	81	GLU
1	I	88	SER
1	I	89	GLN
1	I	94	ARG
1	I	110	GLN
1	I	118	THR
1	I	123	THR
1	I	152	ARG
1	I	164	GLN
1	I	170	LEU
1	I	173	TYR
1	I	183	VAL
1	I	195	ASP
1	I	216	LEU
1	I	217	ASN
1	I	224	GLU
1	I	226	THR
1	I	231	ASN
1	I	245	PRO
1	I	258	ARG
1	I	274	MET
1	I	291	LEU
1	I	295	TRP
1	I	300	SER
1	I	303	ARG
1	I	310	LEU
1	I	321	GLU
1	I	325	GLU
1	I	329	LYS
1	I	330	ARG
1	J	2	HIS
1	J	3	ARG
1	J	50	ASN
1	J	51	THR
1	J	67	SER
1	J	68	SER
1	J	72	SER

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Mol	Chain	Res	Type
1	J	81	GLU
1	J	94	ARG
1	J	115	LEU
1	J	118	THR
1	J	123	THR
1	J	131	SER
1	J	173	TYR
1	J	188	PRO
1	J	193	ASP
1	J	195	ASP
1	J	207	LYS
1	J	214	LYS
1	J	216	LEU
1	J	226	THR
1	J	231	ASN
1	J	244	THR
1	J	245	PRO
1	J	257	HIS
1	J	258	ARG
1	J	267	ILE
1	J	291	LEU
1	J	295	TRP
1	J	298	SER
1	J	310	LEU
1	J	325	GLU
1	J	328	MET
1	J	345	THR
1	J	355	SER
1	K	10	GLU
1	K	25	ASN
1	K	44	GLN
1	K	51	THR
1	K	68	SER
1	K	81	GLU
1	K	94	ARG
1	K	99	GLU
1	K	109	ASP
1	K	115	LEU
1	K	118	THR
1	K	123	THR
1	K	131	SER
1	K	139	LYS

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Mol	Chain	Res	Type
1	K	146	LYS
1	K	152	ARG
1	K	195	ASP
1	K	216	LEU
1	K	226	THR
1	K	237	HIS
1	K	244	THR
1	K	257	HIS
1	K	258	ARG
1	K	291	LEU
1	K	295	TRP
1	K	298	SER
1	K	303	ARG
1	K	308	SER
1	K	310	LEU
1	K	325	GLU
1	K	330	ARG
1	K	348	SER
1	K	353	THR
1	K	354	GLN
1	L	3	ARG
1	L	9	GLN
1	L	10	GLU
1	L	20	GLN
1	L	21	SER
1	L	25	ASN
1	L	51	THR
1	L	69	ILE
1	L	87	ASP
1	L	89	GLN
1	L	115	LEU
1	L	118	THR
1	L	123	THR
1	L	151	LEU
1	L	164	GLN
1	L	173	TYR
1	L	195	ASP
1	L	199	GLU
1	L	200	HIS
1	L	207	LYS
1	L	217	ASN
1	L	226	THR

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Mol	Chain	Res	Type
1	L	237	HIS
1	L	250	MET
1	L	258	ARG
1	L	267	ILE
1	L	291	LEU
1	L	295	TRP
1	L	303	ARG
1	L	310	LEU
1	L	325	GLU
1	L	329	LYS
1	L	330	ARG
1	L	339	LYS
1	L	343	VAL
1	L	344	HIS
1	M	2	HIS
1	M	25	ASN
1	M	51	THR
1	M	69	ILE
1	M	70	ASN
1	M	81	GLU
1	M	109	ASP
1	M	115	LEU
1	M	118	THR
1	M	123	THR
1	M	160	SER
1	M	173	TYR
1	M	191	ILE
1	M	195	ASP
1	M	199	GLU
1	M	200	HIS
1	M	216	LEU
1	M	224	GLU
1	M	226	THR
1	M	244	THR
1	M	245	PRO
1	M	257	HIS
1	M	291	LEU
1	M	295	TRP
1	M	303	ARG
1	M	345	THR
1	M	352	SER
1	M	353	THR

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Mol	Chain	Res	Type
1	M	354	GLN
1	M	355	SER
1	M	356	LEU
1	N	3	ARG
1	N	10	GLU
1	N	16	SER
1	N	44	GLN
1	N	45	ARG
1	N	50	ASN
1	N	51	THR
1	N	65	VAL
1	N	69	ILE
1	N	81	GLU
1	N	82	THR
1	N	89	GLN
1	N	94	ARG
1	N	118	THR
1	N	146	LYS
1	N	152	ARG
1	N	173	TYR
1	N	183	VAL
1	N	193	ASP
1	N	195	ASP
1	N	200	HIS
1	N	216	LEU
1	N	217	ASN
1	N	234	THR
1	N	237	HIS
1	N	257	HIS
1	N	258	ARG
1	N	267	ILE
1	N	291	LEU
1	N	295	TRP
1	N	310	LEU
1	N	316	LYS
1	N	325	GLU
1	N	328	MET
1	O	3	ARG
1	O	9	GLN
1	O	10	GLU
1	O	25	ASN
1	O	27	LYS

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Mol	Chain	Res	Type
1	O	44	GLN
1	O	45	ARG
1	O	51	THR
1	O	67	SER
1	O	70	ASN
1	O	81	GLU
1	O	98	LYS
1	O	107	LYS
1	O	118	THR
1	O	123	THR
1	O	146	LYS
1	O	164	GLN
1	O	173	TYR
1	O	199	GLU
1	O	200	HIS
1	O	244	THR
1	O	245	PRO
1	O	258	ARG
1	O	267	ILE
1	O	270	LEU
1	O	291	LEU
1	O	295	TRP
1	O	296	LYS
1	O	303	ARG
1	O	310	LEU
1	O	325	GLU
1	O	330	ARG
1	O	339	LYS
1	P	3	ARG
1	P	44	GLN
1	P	45	ARG
1	P	49	GLU
1	P	51	THR
1	P	67	SER
1	P	81	GLU
1	P	82	THR
1	P	87	ASP
1	P	100	LYS
1	P	109	ASP
1	P	115	LEU
1	P	118	THR
1	P	123	THR

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Mol	Chain	Res	Type
1	P	146	LYS
1	P	152	ARG
1	P	173	TYR
1	P	199	GLU
1	P	216	LEU
1	P	230	PRO
1	P	244	THR
1	P	257	HIS
1	P	258	ARG
1	P	295	TRP
1	P	310	LEU
1	P	343	VAL
1	P	348	SER
1	P	352	SER
1	P	354	GLN
1	P	355	SER
1	P	356	LEU
1	P	358	THR
1	Q	16	SER
1	Q	45	ARG
1	Q	50	ASN
1	Q	51	THR
1	Q	88	SER
1	Q	89	GLN
1	Q	98	LYS
1	Q	107	LYS
1	Q	115	LEU
1	Q	118	THR
1	Q	123	THR
1	Q	125	GLN
1	Q	131	SER
1	Q	146	LYS
1	Q	164	GLN
1	Q	173	TYR
1	Q	199	GLU
1	Q	216	LEU
1	Q	217	ASN
1	Q	226	THR
1	Q	231	ASN
1	Q	250	MET
1	Q	258	ARG
1	Q	267	ILE

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Mol	Chain	Res	Type
1	Q	291	LEU
1	Q	295	TRP
1	Q	303	ARG
1	Q	310	LEU
1	Q	325	GLU
1	Q	330	ARG
1	Q	344	HIS
1	R	3	ARG
1	R	45	ARG
1	R	51	THR
1	R	70	ASN
1	R	81	GLU
1	R	98	LYS
1	R	115	LEU
1	R	118	THR
1	R	123	THR
1	R	131	SER
1	R	139	LYS
1	R	146	LYS
1	R	152	ARG
1	R	164	GLN
1	R	173	TYR
1	R	199	GLU
1	R	200	HIS
1	R	214	LYS
1	R	216	LEU
1	R	226	THR
1	R	230	PRO
1	R	237	HIS
1	R	244	THR
1	R	245	PRO
1	R	257	HIS
1	R	290	PRO
1	R	291	LEU
1	R	295	TRP
1	R	310	LEU
1	R	316	LYS
1	R	330	ARG
1	R	344	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	80	HIS
1	A	125	GLN
1	A	156	GLN
1	A	179	GLN
1	A	220	HIS
1	A	231	ASN
1	A	287	ASN
1	B	50	ASN
1	B	80	HIS
1	B	89	GLN
1	B	125	GLN
1	B	136	GLN
1	B	179	GLN
1	B	217	ASN
1	B	219	HIS
1	B	220	HIS
1	B	231	ASN
1	C	50	ASN
1	C	80	HIS
1	C	125	GLN
1	C	200	HIS
1	C	231	ASN
1	C	324	GLN
1	D	50	ASN
1	D	70	ASN
1	D	80	HIS
1	D	89	GLN
1	D	125	GLN
1	D	179	GLN
1	D	220	HIS
1	D	231	ASN
1	D	287	ASN
1	E	2	HIS
1	E	9	GLN
1	E	50	ASN
1	E	80	HIS
1	E	125	GLN
1	E	136	GLN
1	E	200	HIS
1	E	220	HIS
1	E	231	ASN
1	E	287	ASN

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Mol	Chain	Res	Type
1	F	50	ASN
1	F	80	HIS
1	F	125	GLN
1	F	136	GLN
1	F	179	GLN
1	F	200	HIS
1	F	231	ASN
1	F	287	ASN
1	G	50	ASN
1	G	70	ASN
1	G	80	HIS
1	G	125	GLN
1	G	136	GLN
1	G	217	ASN
1	G	220	HIS
1	G	231	ASN
1	G	247	GLN
1	G	287	ASN
1	H	50	ASN
1	H	70	ASN
1	H	80	HIS
1	H	125	GLN
1	H	136	GLN
1	H	179	GLN
1	H	200	HIS
1	H	220	HIS
1	H	231	ASN
1	I	50	ASN
1	I	70	ASN
1	I	80	HIS
1	I	89	GLN
1	I	125	GLN
1	I	200	HIS
1	I	217	ASN
1	I	231	ASN
1	J	2	HIS
1	J	50	ASN
1	J	80	HIS
1	J	125	GLN
1	J	136	GLN
1	J	179	GLN
1	J	217	ASN

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Mol	Chain	Res	Type
1	J	231	ASN
1	J	247	GLN
1	J	287	ASN
1	K	50	ASN
1	K	80	HIS
1	K	85	GLN
1	K	125	GLN
1	K	136	GLN
1	K	179	GLN
1	K	200	HIS
1	K	231	ASN
1	K	287	ASN
1	L	50	ASN
1	L	80	HIS
1	L	89	GLN
1	L	125	GLN
1	L	136	GLN
1	L	179	GLN
1	L	200	HIS
1	L	217	ASN
1	L	220	HIS
1	L	231	ASN
1	L	287	ASN
1	M	20	GLN
1	M	50	ASN
1	M	70	ASN
1	M	80	HIS
1	M	89	GLN
1	M	125	GLN
1	M	179	GLN
1	M	231	ASN
1	M	287	ASN
1	M	354	GLN
1	N	50	ASN
1	N	80	HIS
1	N	89	GLN
1	N	156	GLN
1	N	200	HIS
1	N	217	ASN
1	N	231	ASN
1	N	284	ASN
1	N	287	ASN

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Mol	Chain	Res	Type
1	N	344	HIS
1	O	50	ASN
1	O	70	ASN
1	O	80	HIS
1	O	125	GLN
1	O	200	HIS
1	O	220	HIS
1	O	231	ASN
1	O	287	ASN
1	O	324	GLN
1	P	50	ASN
1	P	80	HIS
1	P	125	GLN
1	P	179	GLN
1	P	231	ASN
1	P	287	ASN
1	Q	50	ASN
1	Q	80	HIS
1	Q	125	GLN
1	Q	156	GLN
1	Q	168	ASN
1	Q	217	ASN
1	Q	220	HIS
1	Q	231	ASN
1	R	50	ASN
1	R	70	ASN
1	R	80	HIS
1	R	125	GLN
1	R	220	HIS
1	R	231	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.77	0	6,6,6	1.05	0
2	SO4	A	402	-	4,4,4	1.00	0	6,6,6	1.11	1 (16%)
2	SO4	D	400	-	4,4,4	1.55	2 (50%)	6,6,6	3.04	3 (50%)
2	SO4	E	400	-	4,4,4	1.00	0	6,6,6	0.40	0
2	SO4	G	401	-	4,4,4	1.30	1 (25%)	6,6,6	0.41	0
2	SO4	G	402	-	4,4,4	0.81	0	6,6,6	0.91	0
2	SO4	G	403	-	4,4,4	0.67	0	6,6,6	0.73	0
2	SO4	J	400	-	4,4,4	0.91	0	6,6,6	0.61	0
2	SO4	K	400	-	4,4,4	1.22	1 (25%)	6,6,6	1.27	0
2	SO4	M	401	-	4,4,4	0.75	0	6,6,6	1.16	0
2	SO4	O	401	-	4,4,4	0.73	0	6,6,6	0.70	0
2	SO4	P	401	-	4,4,4	1.06	0	6,6,6	1.31	2 (33%)
2	SO4	P	402	-	4,4,4	0.55	0	6,6,6	0.53	0
2	SO4	R	401	-	4,4,4	1.08	0	6,6,6	1.58	1 (16%)
2	SO4	R	402	-	4,4,4	0.67	0	6,6,6	1.13	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	D	400	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	400	-	-	0/0/0/0	0/0/0/0
2	SO4	G	401	-	-	0/0/0/0	0/0/0/0
2	SO4	G	402	-	-	0/0/0/0	0/0/0/0
2	SO4	G	403	-	-	0/0/0/0	0/0/0/0
2	SO4	J	400	-	-	0/0/0/0	0/0/0/0
2	SO4	K	400	-	-	0/0/0/0	0/0/0/0
2	SO4	M	401	-	-	0/0/0/0	0/0/0/0
2	SO4	O	401	-	-	0/0/0/0	0/0/0/0
2	SO4	P	401	-	-	0/0/0/0	0/0/0/0
2	SO4	P	402	-	-	0/0/0/0	0/0/0/0
2	SO4	R	401	-	-	0/0/0/0	0/0/0/0
2	SO4	R	402	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	SO4	O2-S	2.02	1.56	1.45
2	K	400	SO4	O2-S	2.25	1.57	1.45
2	D	400	SO4	O1-S	2.31	1.58	1.45
2	G	401	SO4	O2-S	2.34	1.58	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	SO4	O4-S-O3	-3.22	94.46	108.96
2	D	400	SO4	O4-S-O2	-2.74	94.16	109.26
2	A	402	SO4	O4-S-O1	-2.29	96.66	109.26
2	P	401	SO4	O4-S-O3	-2.15	99.27	108.96
2	R	402	SO4	O4-S-O3	2.07	118.28	108.96
2	P	401	SO4	O3-S-O2	2.25	121.67	109.26
2	R	401	SO4	O4-S-O3	3.02	122.56	108.96
2	D	400	SO4	O4-S-O1	6.05	142.60	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	SO4	2	0
2	R	402	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.