



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:27 PM UTC

PDB ID : 1E0U / pdb_00001e0u
Title : Structure R271L mutant of E. coli pyruvate kinase
Authors : Fortin, R.; Mattevi, A.
Deposited on : 2000-04-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

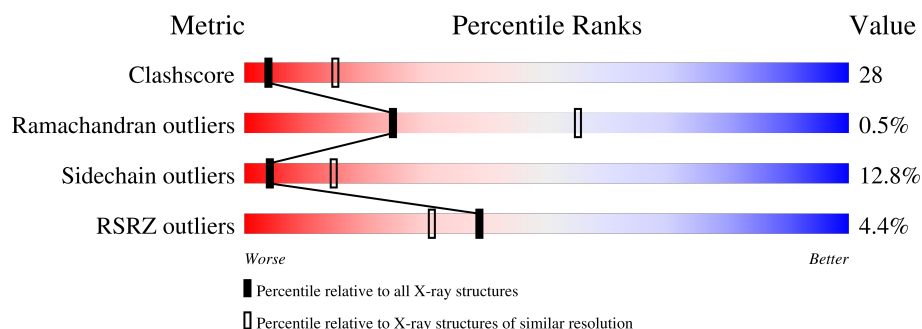
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	470	3% 29% 45% 21% . .
1	B	470	% 28% 44% 23% . .
1	C	470	13% 32% 37% 25% 5% .
1	D	470	26% 46% 24% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14000 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			
1	B	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			
1	C	461	Total	C	N	O	S	11	0	0
			3445	2150	594	676	25			
1	D	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
A	279	MET	GLN	engineered mutation	UNP A0A0A0G552
B	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
B	279	MET	GLN	engineered mutation	UNP A0A0A0G552
C	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
C	279	MET	GLN	engineered mutation	UNP A0A0A0G552
D	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
D	279	MET	GLN	engineered mutation	UNP A0A0A0G552

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

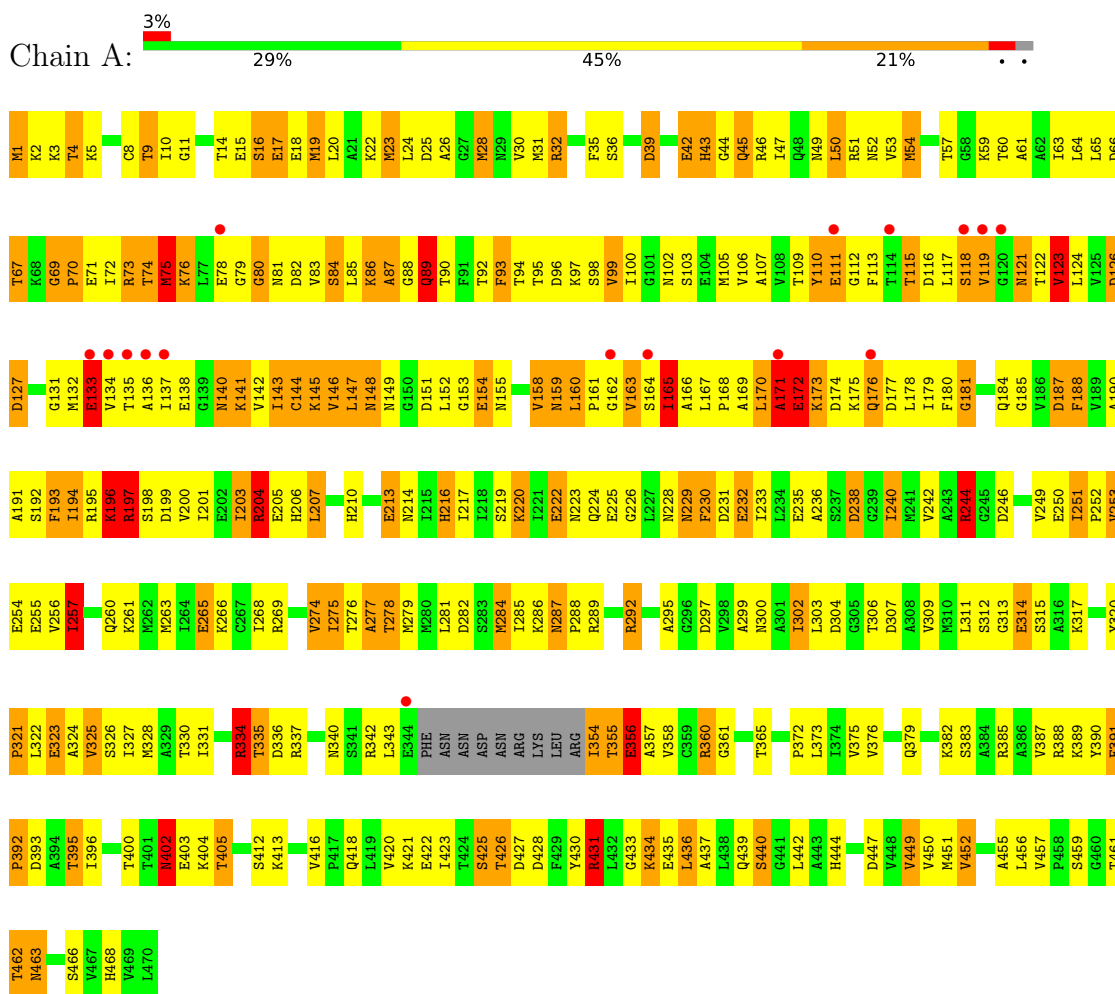
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	55	Total	O	0	0
			55	55		
3	C	48	Total	O	0	0
			48	48		
3	D	59	Total	O	0	0
			59	59		

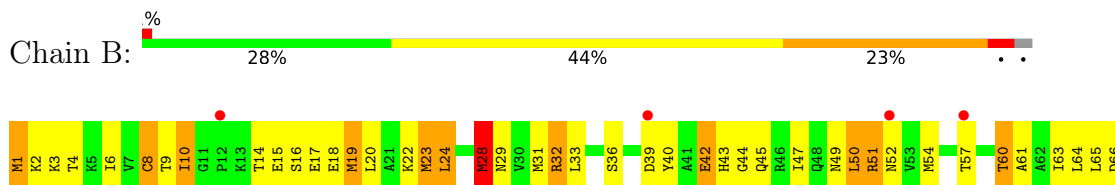
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

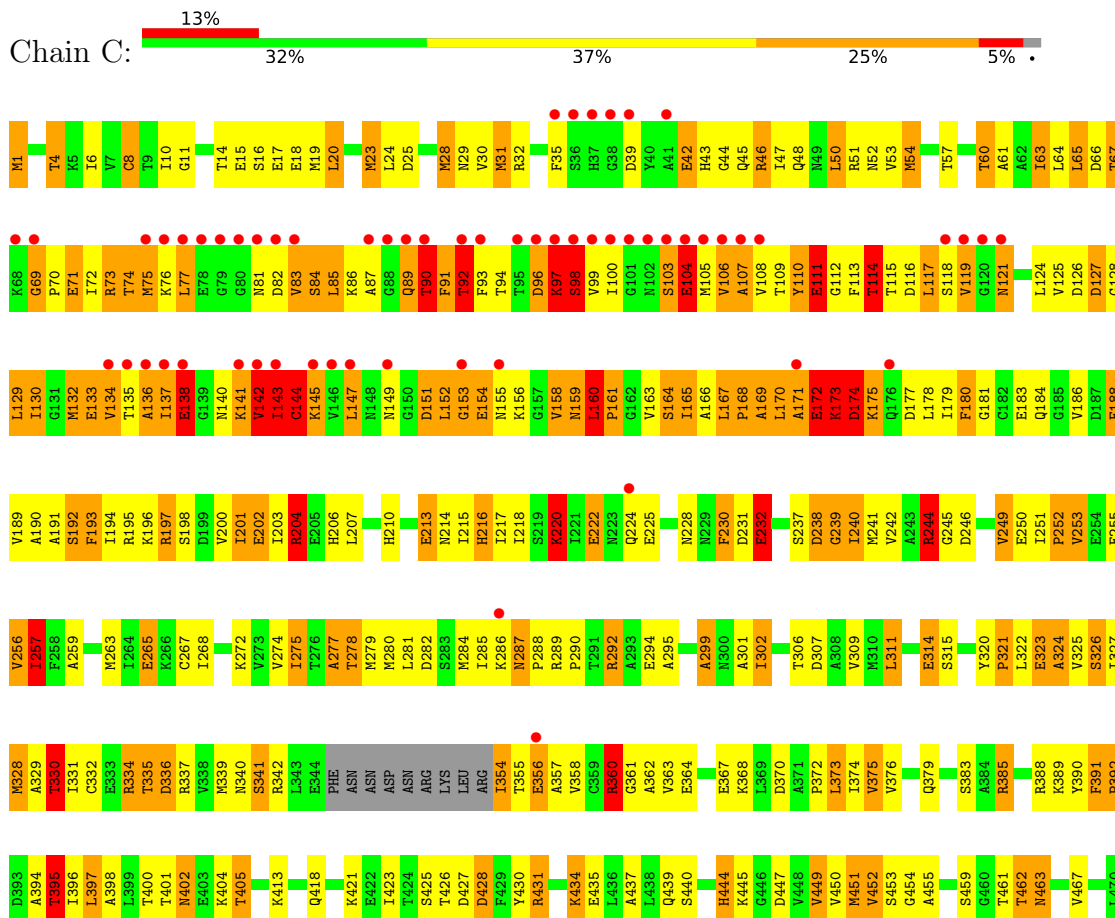
• Molecule 1: Pyruvate kinase



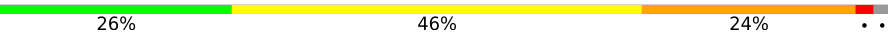
• Molecule 1: Pyruvate kinase

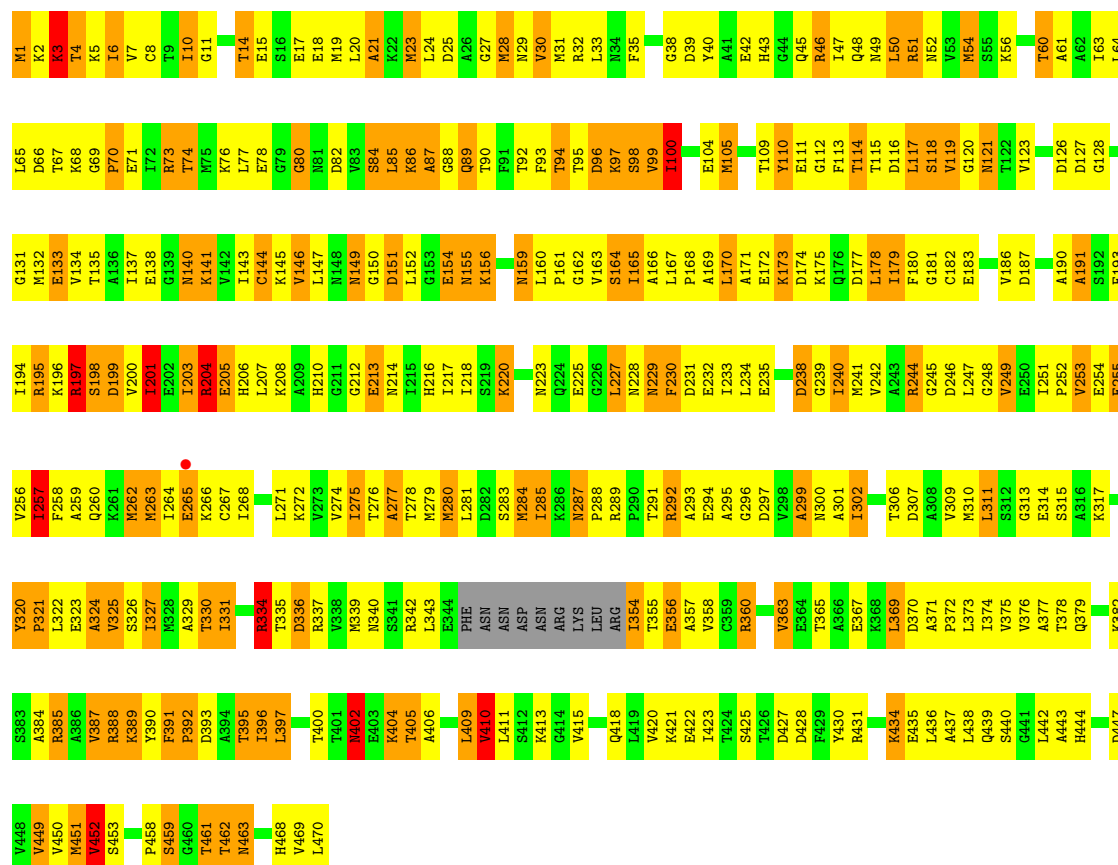


- Molecule 1: Pyruvate kinase



● Molecule 1: Pyruvate kinase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.01Å 129.59Å 241.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.80) 97.2 (15.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.83 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.245 , 0.312 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14000	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1649e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.24	7/3479 (0.2%)	2.97	387/4695 (8.2%)
1	B	1.32	13/3479 (0.4%)	3.03	409/4695 (8.7%)
1	C	1.95	18/3479 (0.5%)	3.18	416/4695 (8.9%)
1	D	1.34	11/3479 (0.3%)	3.06	451/4695 (9.6%)
All	All	1.49	49/13916 (0.4%)	3.06	1663/18780 (8.9%)

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	2
1	B	0	4
1	C	0	3
1	D	0	5
All	All	0	14

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	LYS	CD-CE	65.92	3.50	1.52
1	C	138	GLU	CD-OE1	47.19	2.15	1.25
1	C	111	GLU	CD-OE2	29.23	1.80	1.25
1	C	43	HIS	CE1-NE2	-12.36	1.20	1.32
1	B	216	HIS	CE1-NE2	-11.12	1.21	1.32
1	B	75	MET	CA-C	-9.56	1.48	1.53
1	A	210	HIS	CE1-NE2	-9.55	1.23	1.32
1	C	43	HIS	CG-ND1	-9.25	1.28	1.38
1	B	216	HIS	CG-ND1	-8.74	1.28	1.38
1	D	278	THR	N-CA	8.62	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	ALA	C-O	7.59	1.33	1.23
1	A	210	HIS	CG-ND1	-7.48	1.30	1.38
1	B	278	THR	N-CA	7.21	1.55	1.45
1	D	329	ALA	CA-CB	-7.11	1.42	1.53
1	C	277	ALA	C-O	7.05	1.32	1.24
1	A	197	ARG	CA-CB	-7.00	1.41	1.53
1	D	277	ALA	C-O	6.94	1.32	1.24
1	C	278	THR	N-CA	6.58	1.54	1.45
1	C	63	ILE	C-O	-6.53	1.17	1.24
1	C	287	ASN	C-N	-6.47	1.28	1.33
1	C	216	HIS	CE1-NE2	-6.35	1.26	1.32
1	A	244	ARG	NE-CZ	-6.31	1.26	1.33
1	B	277	ALA	CA-C	-6.18	1.47	1.52
1	D	64	LEU	N-CA	-6.11	1.39	1.46
1	C	43	HIS	CG-CD2	-6.05	1.29	1.35
1	D	216	HIS	CE1-NE2	-5.91	1.26	1.32
1	C	391	PHE	C-O	5.89	1.26	1.23
1	B	292	ARG	C-O	-5.87	1.17	1.24
1	D	187	ASP	N-CA	-5.81	1.38	1.46
1	C	274	VAL	C-O	-5.79	1.18	1.24
1	B	291	THR	C-N	-5.73	1.26	1.33
1	C	97	LYS	CE-NZ	-5.64	1.32	1.49
1	B	431	ARG	C-O	-5.64	1.17	1.24
1	A	388	ARG	CD-NE	-5.61	1.38	1.46
1	B	212	GLY	C-N	-5.50	1.26	1.33
1	D	234	LEU	C-O	-5.37	1.17	1.24
1	B	113	PHE	C-O	-5.34	1.17	1.24
1	C	388	ARG	CD-NE	-5.34	1.38	1.46
1	D	411	LEU	N-CA	-5.27	1.39	1.46
1	C	167	LEU	CA-C	-5.24	1.47	1.53
1	B	47	ILE	N-CA	-5.21	1.40	1.46
1	B	223	ASN	C-O	-5.17	1.17	1.23
1	C	202	GLU	C-O	-5.16	1.17	1.24
1	D	159	ASN	CA-C	-5.15	1.46	1.52
1	A	210	HIS	CD2-NE2	-5.14	1.32	1.37
1	C	332	CYS	C-N	-5.14	1.27	1.33
1	A	210	HIS	CG-CD2	-5.13	1.30	1.35
1	D	197	ARG	NE-CZ	5.12	1.38	1.33
1	D	287	ASN	C-N	-5.04	1.29	1.33

All (1663) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	402	ASN	OD1-CG-ND2	-34.92	87.68	122.60
1	C	111	GLU	CB-CG-CD	33.56	169.66	112.60
1	C	385	ARG	CD-NE-CZ	33.43	171.20	124.40
1	A	73	ARG	CD-NE-CZ	27.64	163.09	124.40
1	A	385	ARG	CD-NE-CZ	26.36	161.30	124.40
1	C	145	LYS	CG-CD-CE	-23.89	56.34	111.30
1	C	43	HIS	ND1-CG-CD2	-22.66	83.44	106.10
1	B	216	HIS	CG-CD2-NE2	22.61	129.81	107.20
1	C	402	ASN	CB-CG-ND2	21.07	148.00	116.40
1	A	210	HIS	ND1-CG-CD2	-20.36	85.74	106.10
1	C	43	HIS	CG-CD2-NE2	19.63	126.83	107.20
1	B	447	ASP	CA-CB-CG	18.80	131.40	112.60
1	B	216	HIS	ND1-CG-CD2	-18.44	87.66	106.10
1	A	210	HIS	CG-CD2-NE2	18.22	125.42	107.20
1	C	142	VAL	N-CA-CB	17.54	135.61	111.41
1	D	385	ARG	CD-NE-CZ	16.83	147.96	124.40
1	D	244	ARG	NE-CZ-NH1	16.76	138.26	121.50
1	B	385	ARG	NE-CZ-NH2	-16.65	104.22	119.20
1	B	216	HIS	CE1-NE2-CD2	-15.93	93.07	109.00
1	D	447	ASP	CA-CB-CG	15.87	128.47	112.60
1	D	334	ARG	CD-NE-CZ	15.65	146.31	124.40
1	D	155	ASN	OD1-CG-ND2	15.55	138.15	122.60
1	B	334	ARG	CD-NE-CZ	15.30	145.83	124.40
1	D	265	GLU	OE1-CD-OE2	-15.29	86.20	122.90
1	C	138	GLU	CG-CD-OE1	-15.12	83.61	118.40
1	C	111	GLU	CG-CD-OE1	15.01	152.93	118.40
1	B	336	ASP	CA-CB-CG	14.76	127.36	112.60
1	B	360	ARG	NE-CZ-NH2	-14.62	106.04	119.20
1	D	149	ASN	OD1-CG-ND2	14.59	137.19	122.60
1	C	334	ARG	CD-NE-CZ	14.41	144.57	124.40
1	D	265	GLU	CG-CD-OE1	14.40	151.52	118.40
1	A	342	ARG	NE-CZ-NH2	-14.23	106.39	119.20
1	D	385	ARG	NE-CZ-NH2	-14.04	106.57	119.20
1	A	334	ARG	CD-NE-CZ	13.93	143.90	124.40
1	B	172	GLU	CA-C-O	-13.90	106.03	120.90
1	B	385	ARG	CD-NE-CZ	13.64	143.50	124.40
1	A	265	GLU	OE1-CD-OE2	-13.57	90.34	122.90
1	C	447	ASP	CA-CB-CG	13.39	125.99	112.60
1	C	342	ARG	NE-CZ-NH2	-13.25	107.28	119.20
1	B	277	ALA	N-CA-C	13.13	130.91	111.34
1	D	145	LYS	CA-CB-CG	13.01	140.11	114.10
1	B	66	ASP	CA-C-O	-12.98	106.47	120.36
1	D	52	ASN	CA-CB-CG	-12.95	99.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	HIS	CB-CG-ND1	12.89	142.04	122.70
1	B	170	LEU	CA-C-O	12.82	135.60	121.11
1	A	52	ASN	CA-CB-CG	-12.68	99.92	112.60
1	B	52	ASN	CA-CB-CG	-12.66	99.94	112.60
1	C	265	GLU	OE1-CD-OE2	-12.66	92.52	122.90
1	B	123	VAL	CA-C-O	-12.60	106.36	120.72
1	A	342	ARG	NE-CZ-NH1	12.57	134.07	121.50
1	C	138	GLU	OE1-CD-OE2	-12.46	93.00	122.90
1	A	72	ILE	CA-C-O	-12.38	107.28	120.53
1	B	277	ALA	O-C-N	-12.37	109.67	121.79
1	B	342	ARG	NE-CZ-NH2	-12.36	108.07	119.20
1	C	43	HIS	CB-CG-ND1	12.28	141.12	122.70
1	B	265	GLU	OE1-CD-OE2	-12.27	93.45	122.90
1	D	357	ALA	O-C-N	12.24	134.68	122.07
1	C	52	ASN	CA-CB-CG	-12.23	100.37	112.60
1	B	342	ARG	CD-NE-CZ	12.18	141.45	124.40
1	A	238	ASP	CA-CB-CG	-12.13	100.47	112.60
1	A	210	HIS	CB-CG-ND1	12.11	140.86	122.70
1	C	138	GLU	CB-CG-CD	12.01	133.02	112.60
1	C	106	VAL	N-CA-CB	11.98	130.20	112.35
1	B	32	ARG	NH1-CZ-NH2	-11.98	103.73	119.30
1	C	197	ARG	NE-CZ-NH1	-11.97	109.53	121.50
1	C	1	MET	CA-CB-CG	11.95	138.01	114.10
1	A	265	GLU	CG-CD-OE1	11.94	145.86	118.40
1	D	360	ARG	NE-CZ-NH2	-11.93	108.47	119.20
1	A	268	ILE	O-C-N	11.92	133.43	121.87
1	D	360	ARG	NE-CZ-NH1	11.91	133.41	121.50
1	A	268	ILE	CA-C-O	-11.90	108.57	120.95
1	D	292	ARG	NE-CZ-NH2	-11.90	108.49	119.20
1	D	66	ASP	CA-C-O	-11.90	107.85	120.58
1	C	18	GLU	O-C-N	11.82	134.65	122.12
1	C	277	ALA	O-C-N	-11.77	106.94	122.59
1	B	224	GLN	CA-C-O	-11.75	107.94	120.63
1	D	463	ASN	OD1-CG-ND2	-11.71	110.89	122.60
1	B	32	ARG	NE-CZ-NH1	11.69	133.19	121.50
1	A	66	ASP	CA-C-O	-11.63	107.92	120.36
1	A	190	ALA	CA-C-O	-11.62	107.54	120.32
1	C	164	SER	N-CA-CB	11.60	129.30	110.16
1	A	190	ALA	O-C-N	11.59	136.94	123.27
1	B	244	ARG	NE-CZ-NH1	11.57	133.07	121.50
1	D	204	ARG	NE-CZ-NH2	11.56	129.60	119.20
1	B	444	HIS	CA-CB-CG	-11.41	102.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	CA-CB-CG	11.36	136.81	114.10
1	C	111	GLU	CA-CB-CG	11.30	136.71	114.10
1	B	360	ARG	NE-CZ-NH1	11.27	132.77	121.50
1	C	216	HIS	ND1-CG-CD2	-11.25	94.85	106.10
1	D	469	VAL	CA-C-O	-11.24	108.54	120.57
1	B	1	MET	CA-CB-CG	11.22	136.55	114.10
1	B	197	ARG	NE-CZ-NH2	11.16	129.25	119.20
1	C	342	ARG	CD-NE-CZ	11.16	140.03	124.40
1	C	256	VAL	CA-C-O	-11.14	109.46	121.05
1	C	342	ARG	NE-CZ-NH1	11.08	132.58	121.50
1	A	159	ASN	OD1-CG-ND2	11.07	133.67	122.60
1	D	277	ALA	N-CA-C	11.06	134.35	110.80
1	C	159	ASN	OD1-CG-ND2	-10.95	111.65	122.60
1	B	155	ASN	OD1-CG-ND2	10.92	133.52	122.60
1	C	143	ILE	N-CA-CB	-10.86	97.78	111.46
1	D	253	VAL	CB-CA-C	-10.81	97.55	112.14
1	C	149	ASN	OD1-CG-ND2	-10.81	111.79	122.60
1	C	43	HIS	CG-ND1-CE1	10.80	127.65	109.30
1	B	204	ARG	NE-CZ-NH2	10.70	128.83	119.20
1	B	287	ASN	OD1-CG-ND2	-10.69	111.91	122.60
1	D	186	VAL	O-C-N	-10.69	113.24	122.65
1	D	342	ARG	NE-CZ-NH2	-10.69	109.58	119.20
1	A	403	GLU	O-C-N	10.61	134.24	122.15
1	C	238	ASP	CA-CB-CG	-10.59	102.01	112.60
1	B	277	ALA	CA-C-O	-10.59	107.75	119.40
1	D	453	SER	CA-C-N	10.59	132.57	122.73
1	D	453	SER	C-N-CA	10.59	132.57	122.73
1	B	180	PHE	O-C-N	10.50	132.88	122.07
1	A	342	ARG	CD-NE-CZ	10.49	139.09	124.40
1	C	357	ALA	O-C-N	10.48	134.10	122.15
1	D	150	GLY	CA-C-O	-10.47	111.36	121.62
1	A	197	ARG	N-CA-CB	-10.47	94.10	110.22
1	B	123	VAL	O-C-N	10.46	133.81	123.14
1	B	230	PHE	CA-CB-CG	-10.33	103.47	113.80
1	D	342	ARG	CD-NE-CZ	10.27	138.78	124.40
1	B	224	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	D	199	ASP	CA-CB-CG	10.24	122.84	112.60
1	B	167	LEU	CA-C-O	10.23	132.25	120.69
1	C	361	GLY	O-C-N	10.23	132.12	122.19
1	D	45	GLN	OE1-CD-NE2	10.22	132.82	122.60
1	C	8	CYS	CA-C-O	-10.20	109.34	120.36
1	A	427	ASP	CA-CB-CG	10.19	122.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ASP	CA-CB-CG	10.19	122.79	112.60
1	D	287	ASN	OD1-CG-ND2	-10.13	112.47	122.60
1	D	244	ARG	CA-CB-CG	-10.12	93.86	114.10
1	B	6	ILE	O-C-N	10.05	133.85	123.20
1	C	295	ALA	CA-C-O	-10.04	109.91	120.55
1	B	44	GLY	O-C-N	10.03	131.92	122.19
1	C	104	GLU	CG-CD-OE1	-9.99	95.42	118.40
1	A	236	ALA	CA-C-O	-9.97	108.02	119.79
1	C	110	TYR	CA-C-O	9.97	133.13	120.57
1	C	265	GLU	CG-CD-OE2	9.90	141.17	118.40
1	A	277	ALA	O-C-N	-9.87	109.46	122.59
1	C	249	VAL	CA-C-O	9.84	131.15	120.32
1	D	311	LEU	CA-C-O	9.84	132.23	120.92
1	A	277	ALA	N-CA-C	9.83	131.74	110.80
1	A	121	ASN	CA-CB-CG	9.82	122.42	112.60
1	D	238	ASP	N-CA-C	-9.82	100.80	113.17
1	C	361	GLY	CA-C-O	-9.78	110.29	120.66
1	C	214	ASN	OD1-CG-ND2	-9.74	112.86	122.60
1	D	295	ALA	CA-C-O	-9.71	110.15	120.63
1	D	82	ASP	CA-C-O	-9.68	111.29	121.55
1	D	395	THR	CA-CB-OG1	-9.68	95.08	109.60
1	C	280	MET	CA-C-O	-9.64	110.11	120.71
1	C	289	ARG	O-C-N	9.63	128.59	121.85
1	B	264	ILE	O-C-N	-9.61	112.49	121.91
1	C	174	ASP	N-CA-C	-9.60	100.80	111.07
1	A	99	VAL	CA-C-O	9.59	131.91	121.36
1	C	127	ASP	CA-CB-CG	9.58	122.18	112.60
1	A	164	SER	CA-C-O	-9.56	109.72	120.43
1	B	155	ASN	CA-CB-CG	-9.56	103.04	112.60
1	D	299	ALA	N-CA-CB	-9.55	96.08	110.12
1	C	224	GLN	OE1-CD-NE2	-9.53	113.08	122.60
1	C	161	PRO	CB-CA-C	9.49	123.70	111.46
1	A	78	GLU	CB-CG-CD	9.47	128.71	112.60
1	C	463	ASN	OD1-CG-ND2	-9.45	113.15	122.60
1	C	43	HIS	CE1-NE2-CD2	-9.45	99.55	109.00
1	D	86	LYS	CA-C-O	9.45	130.56	120.36
1	B	273	VAL	O-C-N	9.43	130.95	122.65
1	A	102	ASN	OD1-CG-ND2	9.43	132.03	122.60
1	C	437	ALA	CA-C-O	9.42	130.71	120.82
1	B	342	ARG	NE-CZ-NH1	9.40	130.90	121.50
1	C	278	THR	N-CA-CB	-9.38	97.49	110.25
1	A	111	GLU	N-CA-CB	-9.37	93.31	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	ALA	O-C-N	-9.35	110.16	122.59
1	A	210	HIS	CG-ND1-CE1	9.32	125.15	109.30
1	B	469	VAL	CA-C-O	-9.31	110.61	120.57
1	B	199	ASP	O-C-N	-9.30	112.49	122.07
1	B	228	ASN	CA-CB-CG	9.29	121.89	112.60
1	B	105	MET	CA-CB-CG	9.26	132.62	114.10
1	B	392	PRO	CA-C-O	-9.26	111.06	121.43
1	D	143	ILE	CA-CB-CG2	9.23	126.19	110.50
1	D	265	GLU	CA-C-O	-9.20	111.16	120.82
1	A	326	SER	CA-C-O	-9.20	110.80	120.55
1	C	61	ALA	CA-C-O	-9.19	111.62	121.36
1	C	181	GLY	CA-C-O	9.17	129.79	120.80
1	B	265	GLU	CG-CD-OE2	9.16	139.46	118.40
1	C	66	ASP	CA-C-O	-9.15	110.19	120.43
1	B	86	LYS	CA-C-O	9.13	130.46	120.32
1	B	148	ASN	CA-CB-CG	9.12	121.72	112.60
1	B	170	LEU	O-C-N	-9.12	111.34	123.19
1	B	87	ALA	CA-C-O	-9.11	111.13	121.15
1	A	306	THR	O-C-N	-9.06	112.15	122.75
1	D	307	ASP	CA-CB-CG	9.06	121.66	112.60
1	A	172	GLU	N-CA-C	9.06	120.92	111.14
1	D	119	VAL	N-CA-CB	9.03	121.97	110.05
1	B	414	GLY	CA-C-N	-9.03	110.00	122.91
1	B	414	GLY	C-N-CA	-9.03	110.00	122.91
1	B	274	VAL	CA-C-O	9.01	130.67	120.76
1	D	1	MET	CA-CB-CG	9.01	132.11	114.10
1	A	169	ALA	CA-C-O	8.99	129.95	120.42
1	A	149	ASN	CA-C-O	-8.98	111.10	121.16
1	A	207	LEU	O-C-N	8.97	131.42	122.09
1	A	337	ARG	NE-CZ-NH2	-8.95	111.15	119.20
1	D	256	VAL	CA-C-O	-8.93	111.76	121.05
1	B	49	ASN	O-C-N	8.92	132.65	122.22
1	C	124	LEU	CA-C-O	-8.90	111.27	120.71
1	A	66	ASP	CA-CB-CG	-8.90	103.70	112.60
1	B	105	MET	O-C-N	8.89	132.27	123.46
1	B	460	GLY	CA-C-O	8.88	128.55	118.96
1	A	285	ILE	N-CA-C	-8.88	99.99	111.09
1	B	268	ILE	CA-C-O	-8.87	111.77	121.17
1	B	254	GLU	CA-C-O	-8.86	107.94	119.10
1	C	106	VAL	CA-C-O	8.84	130.31	121.64
1	D	155	ASN	CA-CB-CG	-8.81	103.79	112.60
1	A	26	ALA	CA-C-O	-8.81	107.83	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	LEU	CA-C-O	8.81	130.03	120.43
1	C	277	ALA	N-CA-C	8.80	129.55	110.80
1	C	244	ARG	NE-CZ-NH2	-8.80	111.28	119.20
1	A	42	GLU	N-CA-CB	8.78	122.81	110.07
1	A	216	HIS	ND1-CG-CD2	-8.78	97.32	106.10
1	C	214	ASN	CA-CB-CG	8.78	121.38	112.60
1	D	331	ILE	CB-CA-C	-8.78	100.52	112.02
1	B	61	ALA	CA-C-O	-8.78	112.06	121.36
1	B	463	ASN	OD1-CG-ND2	-8.78	113.82	122.60
1	B	292	ARG	NE-CZ-NH2	-8.77	111.31	119.20
1	D	179	ILE	CB-CG1-CD1	8.75	132.18	113.80
1	C	172	GLU	CB-CG-CD	8.75	127.47	112.60
1	C	395	THR	CA-CB-OG1	-8.75	96.48	109.60
1	B	250	GLU	CA-C-O	8.74	128.76	119.14
1	A	361	GLY	CA-C-O	-8.74	111.56	121.00
1	D	97	LYS	N-CA-CB	-8.72	95.76	110.49
1	A	231	ASP	CA-C-N	-8.71	107.06	120.31
1	A	231	ASP	C-N-CA	-8.71	107.06	120.31
1	A	253	VAL	CB-CA-C	-8.70	100.74	111.88
1	C	335	THR	CA-C-O	8.70	129.90	120.24
1	D	356	GLU	CB-CG-CD	8.70	127.39	112.60
1	D	45	GLN	CA-C-O	8.69	129.63	120.42
1	B	64	LEU	CA-C-O	8.68	129.74	120.36
1	D	248	GLY	CA-C-N	8.67	131.64	121.84
1	D	248	GLY	C-N-CA	8.67	131.64	121.84
1	B	244	ARG	NH1-CZ-NH2	-8.65	108.05	119.30
1	C	244	ARG	NE-CZ-NH1	8.64	130.14	121.50
1	A	373	LEU	CA-C-N	-8.63	112.49	123.19
1	A	373	LEU	C-N-CA	-8.63	112.49	123.19
1	A	149	ASN	OD1-CG-ND2	8.62	131.22	122.60
1	D	397	LEU	CA-C-O	-8.61	110.78	120.43
1	A	140	ASN	CA-CB-CG	8.61	121.21	112.60
1	C	98	SER	CA-CB-OG	8.60	128.30	111.10
1	D	63	ILE	CA-C-N	8.58	135.05	122.86
1	D	63	ILE	C-N-CA	8.58	135.05	122.86
1	A	134	VAL	N-CA-CB	8.58	120.56	110.95
1	C	73	ARG	CB-CA-C	-8.57	95.02	109.50
1	D	67	THR	N-CA-CB	8.56	122.60	110.36
1	D	140	ASN	N-CA-CB	-8.53	98.53	110.65
1	D	387	VAL	N-CA-C	-8.52	101.71	111.00
1	B	230	PHE	CA-C-N	8.50	132.61	120.79
1	B	230	PHE	C-N-CA	8.50	132.61	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	CA-CB-CG	8.49	131.08	114.10
1	B	256	VAL	CA-C-O	-8.48	112.13	120.95
1	C	207	LEU	CA-C-O	8.48	129.41	120.42
1	C	63	ILE	O-C-N	8.46	131.98	123.18
1	A	256	VAL	CA-C-O	-8.44	112.27	121.05
1	D	299	ALA	N-CA-C	-8.44	102.08	111.28
1	A	61	ALA	CA-C-O	-8.43	112.04	121.40
1	B	199	ASP	CA-CB-CG	8.42	121.02	112.60
1	B	238	ASP	N-CA-C	-8.42	102.57	113.17
1	A	171	ALA	O-C-N	-8.40	111.42	122.59
1	C	274	VAL	CA-C-N	-8.40	112.26	123.10
1	C	274	VAL	C-N-CA	-8.40	112.26	123.10
1	A	69	GLY	CA-C-N	8.38	128.40	119.76
1	A	69	GLY	C-N-CA	8.38	128.40	119.76
1	C	239	GLY	O-C-N	-8.39	115.42	123.81
1	A	274	VAL	CA-C-N	-8.38	111.50	123.06
1	A	274	VAL	C-N-CA	-8.38	111.50	123.06
1	D	400	THR	CA-C-N	-8.38	109.51	122.49
1	D	400	THR	C-N-CA	-8.38	109.51	122.49
1	C	389	LYS	O-C-N	-8.37	112.66	122.20
1	D	233	ILE	CA-C-O	8.36	129.72	120.85
1	A	149	ASN	CA-CB-CG	-8.34	104.27	112.60
1	C	164	SER	CB-CA-C	-8.32	96.15	109.80
1	A	86	LYS	CA-C-O	8.30	129.54	120.32
1	C	165	ILE	CA-C-O	8.29	130.45	120.84
1	C	337	ARG	NE-CZ-NH2	-8.28	111.75	119.20
1	D	400	THR	O-C-N	8.28	132.69	123.25
1	B	98	SER	O-C-N	8.27	133.58	122.49
1	A	277	ALA	CA-C-O	-8.27	108.69	120.51
1	D	244	ARG	NH1-CZ-NH2	-8.27	108.55	119.30
1	C	174	ASP	CB-CA-C	8.25	123.83	110.88
1	B	136	ALA	O-C-N	-8.25	114.24	123.48
1	C	42	GLU	O-C-N	8.24	131.00	122.09
1	D	49	ASN	O-C-N	8.24	130.86	122.12
1	B	461	THR	CB-CA-C	8.24	124.07	109.65
1	C	326	SER	CA-C-O	-8.21	111.85	120.55
1	A	217	ILE	O-C-N	8.19	132.68	123.10
1	D	4	THR	CA-C-O	-8.18	111.60	120.92
1	D	300	ASN	CA-CB-CG	8.17	120.77	112.60
1	D	321	PRO	N-CD-CG	-8.16	90.96	103.20
1	A	354	ILE	N-CA-CB	8.15	125.36	111.50
1	B	15	GLU	CG-CD-OE2	8.14	137.13	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ASP	CA-CB-CG	-8.14	104.46	112.60
1	A	422	GLU	O-C-N	8.14	132.19	123.56
1	B	395	THR	CA-CB-OG1	-8.14	97.39	109.60
1	C	173	LYS	N-CA-C	-8.13	103.49	113.41
1	D	66	ASP	CA-CB-CG	-8.13	104.47	112.60
1	B	292	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	C	50	LEU	O-C-N	8.12	130.73	122.12
1	C	418	GLN	CA-C-O	8.10	131.15	120.21
1	B	163	VAL	CB-CA-C	-8.10	100.12	111.21
1	D	254	GLU	CA-C-O	-8.10	108.52	119.05
1	D	277	ALA	CA-C-O	-8.10	108.93	120.51
1	C	277	ALA	CA-C-O	-8.09	108.94	120.51
1	C	188	PHE	CA-C-N	8.07	133.83	123.10
1	C	188	PHE	C-N-CA	8.07	133.83	123.10
1	D	450	VAL	CA-C-O	-8.07	111.93	120.48
1	A	222	GLU	CB-CG-CD	8.03	126.25	112.60
1	D	161	PRO	N-CA-CB	8.03	110.32	103.25
1	A	173	LYS	CA-C-O	8.03	129.17	120.10
1	C	84	SER	CA-C-O	8.01	129.40	120.43
1	B	146	VAL	O-C-N	8.01	131.40	122.67
1	C	92	THR	N-CA-CB	-8.00	96.65	111.52
1	C	257	ILE	O-C-N	8.00	132.77	121.82
1	A	42	GLU	CB-CG-CD	7.98	126.17	112.60
1	C	143	ILE	CA-C-N	-7.97	109.70	122.53
1	C	143	ILE	C-N-CA	-7.97	109.70	122.53
1	A	123	VAL	CA-C-O	-7.96	112.02	120.53
1	D	249	VAL	CB-CA-C	-7.94	104.07	111.06
1	A	391	PHE	CA-C-O	7.94	125.95	120.47
1	A	232	GLU	OE1-CD-OE2	7.93	141.93	122.90
1	B	173	LYS	CB-CG-CD	7.92	129.52	111.30
1	A	30	VAL	O-C-N	7.92	131.57	123.10
1	A	444	HIS	CA-CB-CG	-7.92	105.89	113.80
1	A	197	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	B	177	ASP	CA-CB-CG	7.91	120.51	112.60
1	B	339	MET	O-C-N	-7.91	113.43	122.68
1	D	170	LEU	N-CA-CB	-7.91	96.81	111.52
1	B	148	ASN	CB-CG-ND2	7.90	128.25	116.40
1	B	251	ILE	O-C-N	7.90	127.25	121.72
1	D	256	VAL	O-C-N	-7.90	114.15	121.89
1	D	235	GLU	O-C-N	7.88	130.48	122.12
1	D	280	MET	CA-C-O	-7.87	112.62	120.89
1	C	111	GLU	OE1-CD-OE2	-7.87	104.01	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	HIS	CE1-NE2-CD2	-7.86	101.14	109.00
1	C	197	ARG	NH1-CZ-NH2	7.86	129.51	119.30
1	C	104	GLU	CG-CD-OE2	7.86	136.47	118.40
1	D	206	HIS	N-CA-CB	-7.85	98.54	110.16
1	B	140	ASN	N-CA-CB	-7.85	99.19	110.57
1	A	335	THR	CA-C-O	7.84	128.94	120.24
1	D	385	ARG	NH1-CZ-NH2	7.84	129.49	119.30
1	B	222	GLU	CB-CG-CD	7.83	125.91	112.60
1	A	360	ARG	NE-CZ-NH2	-7.83	112.15	119.20
1	D	46	ARG	NE-CZ-NH2	-7.83	112.16	119.20
1	D	287	ASN	CA-CB-CG	-7.81	104.79	112.60
1	C	154	GLU	CB-CA-C	7.81	123.66	109.37
1	D	470	LEU	CA-C-O	-7.80	107.54	120.80
1	A	111	GLU	CB-CA-C	7.79	127.63	110.18
1	A	42	GLU	N-CA-C	-7.79	102.73	111.14
1	C	99	VAL	CA-C-O	7.78	129.92	121.36
1	C	111	GLU	CG-CD-OE2	-7.78	100.50	118.40
1	D	249	VAL	N-CA-C	-7.78	105.19	112.96
1	D	439	GLN	CA-C-O	-7.77	111.32	120.10
1	B	343	LEU	CA-C-O	7.77	130.02	120.31
1	C	45	GLN	CG-CD-NE2	7.76	128.04	116.40
1	B	214	ASN	CA-CB-CG	7.76	120.36	112.60
1	C	268	ILE	O-C-N	7.75	129.81	121.83
1	D	64	LEU	CA-C-O	7.75	128.70	120.33
1	C	92	THR	OG1-CB-CG2	7.74	124.78	109.30
1	C	374	ILE	CA-C-N	-7.73	113.60	123.19
1	C	374	ILE	C-N-CA	-7.73	113.60	123.19
1	B	230	PHE	O-C-N	-7.73	112.31	122.59
1	C	159	ASN	CB-CG-ND2	7.73	127.99	116.40
1	A	4	THR	CA-C-O	-7.72	112.12	120.92
1	A	146	VAL	CA-C-O	-7.70	112.26	121.04
1	D	229	ASN	CA-CB-CG	-7.70	104.90	112.60
1	C	92	THR	CB-CA-C	7.70	126.33	109.94
1	A	450	VAL	O-C-N	-7.69	115.05	123.20
1	D	149	ASN	CA-C-O	-7.69	112.55	121.16
1	B	288	PRO	CA-C-O	7.68	127.44	118.68
1	D	259	ALA	CA-C-O	7.68	128.88	120.82
1	A	81	ASN	OD1-CG-ND2	7.67	130.27	122.60
1	A	287	ASN	O-C-N	7.67	127.87	121.35
1	C	405	THR	CB-CA-C	7.67	122.92	110.88
1	D	159	ASN	CA-C-O	-7.67	112.42	120.70
1	B	71	GLU	N-CA-CB	-7.66	98.86	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	PHE	CA-CB-CG	-7.66	106.14	113.80
1	C	400	THR	O-C-N	7.66	131.62	123.42
1	A	78	GLU	CB-CA-C	-7.66	99.42	110.06
1	B	158	VAL	CA-C-O	-7.66	111.71	120.67
1	B	309	VAL	CA-C-N	-7.65	112.20	122.99
1	B	309	VAL	C-N-CA	-7.65	112.20	122.99
1	A	418	GLN	CA-C-O	7.65	130.54	120.21
1	C	299	ALA	CA-C-O	7.65	129.08	120.90
1	C	153	GLY	CA-C-N	-7.64	110.56	122.87
1	C	153	GLY	C-N-CA	-7.64	110.56	122.87
1	A	16	SER	O-C-N	-7.63	113.82	122.75
1	C	96	ASP	CA-CB-CG	7.63	120.23	112.60
1	D	25	ASP	CA-C-O	-7.63	112.80	120.82
1	B	140	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	A	110	TYR	CA-C-O	7.62	130.48	121.11
1	D	218	ILE	CA-C-N	-7.61	110.54	121.42
1	D	218	ILE	C-N-CA	-7.61	110.54	121.42
1	A	75	MET	CA-C-O	7.60	122.35	117.94
1	D	150	GLY	CA-C-N	-7.59	111.92	122.93
1	D	150	GLY	C-N-CA	-7.59	111.92	122.93
1	A	70	PRO	CB-CA-C	-7.59	101.67	111.46
1	B	191	ALA	O-C-N	-7.58	114.58	123.22
1	D	173	LYS	O-C-N	-7.56	113.38	122.22
1	C	357	ALA	CA-C-O	-7.55	112.42	120.42
1	C	451	MET	CA-C-O	-7.53	112.04	120.32
1	D	228	ASN	O-C-N	-7.52	114.15	122.12
1	D	47	ILE	CA-C-O	7.49	128.79	120.85
1	A	3	LYS	N-CA-C	-7.49	104.00	113.43
1	A	242	VAL	CB-CA-C	-7.49	101.90	110.96
1	B	180	PHE	CA-CB-CG	7.49	121.29	113.80
1	C	309	VAL	CA-C-N	-7.48	110.61	122.73
1	C	309	VAL	C-N-CA	-7.48	110.61	122.73
1	B	24	LEU	N-CA-C	-7.47	103.14	111.28
1	A	181	GLY	CA-C-N	-7.47	110.73	120.44
1	A	181	GLY	C-N-CA	-7.47	110.73	120.44
1	B	278	THR	N-CA-CB	-7.45	100.11	110.25
1	C	373	LEU	N-CA-C	7.43	120.59	108.55
1	A	340	ASN	CA-C-O	-7.42	112.75	121.44
1	D	128	GLY	CA-C-N	-7.42	110.79	120.44
1	D	128	GLY	C-N-CA	-7.42	110.79	120.44
1	D	43	HIS	CG-CD2-NE2	7.42	114.62	107.20
1	D	6	ILE	O-C-N	7.40	131.04	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	HIS	ND1-CG-CD2	-7.40	98.70	106.10
1	B	354	ILE	CA-C-N	-7.40	110.55	120.54
1	B	354	ILE	C-N-CA	-7.40	110.55	120.54
1	B	192	SER	CA-CB-OG	7.40	125.89	111.10
1	B	295	ALA	CA-C-O	-7.39	112.71	120.55
1	D	444	HIS	CA-CB-CG	-7.39	106.41	113.80
1	D	247	LEU	CA-C-O	7.38	128.38	120.55
1	A	436	LEU	N-CA-CB	-7.38	99.23	110.16
1	C	202	GLU	CG-CD-OE1	7.37	135.34	118.40
1	B	362	ALA	O-C-N	7.37	129.93	122.12
1	B	169	ALA	N-CA-CB	-7.36	99.30	110.12
1	C	204	ARG	NE-CZ-NH2	7.36	125.83	119.20
1	B	115	THR	CA-CB-CG2	-7.36	97.99	110.50
1	D	164	SER	CB-CA-C	-7.36	97.85	109.84
1	B	253	VAL	CB-CA-C	-7.35	102.41	112.04
1	C	142	VAL	O-C-N	7.35	131.20	123.26
1	C	210	HIS	O-C-N	-7.35	112.34	122.19
1	C	24	LEU	O-C-N	7.34	129.90	122.12
1	D	201	ILE	N-CA-C	7.34	118.11	110.62
1	B	305	GLY	O-C-N	-7.34	114.88	122.51
1	D	342	ARG	NE-CZ-NH1	7.34	128.84	121.50
1	A	249	VAL	N-CA-C	-7.33	105.62	112.96
1	B	320	TYR	CB-CA-C	-7.33	101.73	111.11
1	D	191	ALA	O-C-N	-7.33	114.70	123.13
1	D	311	LEU	O-C-N	-7.33	114.66	123.16
1	C	402	ASN	CA-CB-CG	-7.33	105.27	112.60
1	B	357	ALA	O-C-N	7.32	130.00	122.09
1	D	94	THR	CA-CB-OG1	-7.32	98.62	109.60
1	D	427	ASP	CA-CB-CG	7.31	119.91	112.60
1	D	422	GLU	O-C-N	7.30	131.30	123.56
1	C	444	HIS	CA-CB-CG	-7.30	106.50	113.80
1	B	100	ILE	N-CA-CB	7.30	121.09	111.90
1	D	127	ASP	N-CA-CB	7.30	122.80	111.71
1	B	210	HIS	ND1-CG-CD2	-7.29	98.81	106.10
1	C	249	VAL	N-CA-C	-7.29	105.54	111.81
1	D	264	ILE	O-C-N	-7.29	114.80	121.87
1	A	127	ASP	CA-CB-CG	7.29	119.89	112.60
1	D	180	PHE	CA-CB-CG	7.29	121.08	113.80
1	C	129	LEU	CA-C-O	-7.28	112.50	121.02
1	C	81	ASN	CA-CB-CG	-7.28	105.32	112.60
1	D	119	VAL	CB-CA-C	-7.27	100.22	111.71
1	C	230	PHE	CA-CB-CG	-7.27	106.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	VAL	CB-CA-C	-7.25	103.39	111.23
1	C	216	HIS	CG-CD2-NE2	7.25	114.45	107.20
1	B	265	GLU	CA-C-O	-7.25	113.21	120.82
1	C	111	GLU	N-CA-CB	7.25	122.74	110.49
1	D	3	LYS	CA-C-O	-7.24	111.02	119.78
1	D	187	ASP	CA-CB-CG	7.23	119.83	112.60
1	C	282	ASP	CA-CB-CG	7.22	119.82	112.60
1	C	29	ASN	CA-C-N	-7.21	112.33	122.71
1	C	29	ASN	C-N-CA	-7.21	112.33	122.71
1	A	266	LYS	CA-C-N	-7.20	111.08	120.44
1	A	266	LYS	C-N-CA	-7.20	111.08	120.44
1	C	45	GLN	N-CA-C	-7.20	103.51	111.36
1	C	253	VAL	CA-C-O	7.20	129.78	120.78
1	B	171	ALA	CB-CA-C	7.19	122.53	109.37
1	C	375	VAL	CA-C-N	-7.18	112.96	122.94
1	C	375	VAL	C-N-CA	-7.18	112.96	122.94
1	C	30	VAL	O-C-N	7.18	131.01	123.05
1	A	188	PHE	CA-C-N	7.17	132.54	123.14
1	A	188	PHE	C-N-CA	7.17	132.54	123.14
1	A	95	THR	N-CA-CB	7.16	122.44	110.41
1	D	400	THR	CA-C-O	-7.16	113.60	121.33
1	D	257	ILE	CB-CG1-CD1	-7.15	98.78	113.80
1	D	115	THR	N-CA-CB	-7.15	99.58	110.16
1	C	124	LEU	CA-C-N	-7.14	113.01	122.94
1	C	124	LEU	C-N-CA	-7.14	113.01	122.94
1	C	141	LYS	N-CA-C	7.14	120.83	108.76
1	B	243	ALA	N-CA-CB	-7.14	100.00	110.49
1	D	150	GLY	O-C-N	7.14	131.95	123.67
1	C	373	LEU	CA-C-N	-7.13	114.34	123.19
1	C	373	LEU	C-N-CA	-7.13	114.34	123.19
1	D	410	VAL	O-C-N	-7.13	114.90	121.89
1	D	331	ILE	N-CA-C	-7.13	103.83	110.53
1	D	430	TYR	CA-C-O	-7.13	112.22	120.20
1	A	278	THR	N-CA-CB	-7.12	100.60	110.29
1	C	439	GLN	N-CA-CB	7.12	121.39	110.14
1	D	203	ILE	CA-C-N	-7.12	109.48	120.31
1	D	203	ILE	C-N-CA	-7.12	109.48	120.31
1	D	51	ARG	NH1-CZ-NH2	-7.12	110.04	119.30
1	D	302	ILE	O-C-N	-7.12	114.50	121.83
1	A	337	ARG	NH1-CZ-NH2	7.12	128.55	119.30
1	D	168	PRO	CA-C-N	7.11	130.76	120.38
1	D	168	PRO	C-N-CA	7.11	130.76	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	175	LYS	O-C-N	7.10	131.46	122.23
1	B	197	ARG	NE-CZ-NH1	-7.09	114.41	121.50
1	C	216	HIS	CB-CG-CD2	7.08	140.41	131.20
1	B	270	ALA	CA-C-O	-7.08	110.76	119.18
1	D	123	VAL	CA-CB-CG1	-7.08	98.37	110.40
1	D	371	ALA	CA-C-N	7.08	127.69	120.04
1	D	371	ALA	C-N-CA	7.08	127.69	120.04
1	C	285	ILE	N-CA-C	-7.08	102.14	112.04
1	D	105	MET	O-C-N	7.07	130.46	123.46
1	D	428	ASP	CA-CB-CG	-7.07	105.53	112.60
1	A	292	ARG	CA-CB-CG	7.06	128.22	114.10
1	B	370	ASP	CA-C-O	-7.06	113.39	121.65
1	B	172	GLU	CG-CD-OE1	7.06	134.64	118.40
1	B	279	MET	N-CA-C	7.06	121.14	111.54
1	A	71	GLU	CA-C-O	-7.05	113.72	121.33
1	B	45	GLN	CA-C-O	7.04	127.89	120.42
1	B	180	PHE	CA-C-O	-7.04	113.43	120.82
1	C	6	ILE	CA-C-O	7.04	127.71	120.39
1	A	244	ARG	CD-NE-CZ	7.04	134.25	124.40
1	A	300	ASN	CB-CG-ND2	7.04	126.95	116.40
1	C	42	GLU	N-CA-C	-7.04	103.54	111.14
1	C	232	GLU	OE1-CD-OE2	7.03	139.78	122.90
1	D	360	ARG	O-C-N	7.03	130.16	122.15
1	A	216	HIS	CA-C-O	-7.03	112.73	120.81
1	C	87	ALA	CA-C-O	-7.03	113.85	121.44
1	A	9	THR	CA-C-N	-7.02	114.08	122.93
1	A	9	THR	C-N-CA	-7.02	114.08	122.93
1	B	439	GLN	CA-C-O	-7.02	112.16	120.10
1	D	297	ASP	O-C-N	-7.02	114.79	122.09
1	B	15	GLU	OE1-CD-OE2	-7.02	106.06	122.90
1	D	45	GLN	CG-CD-OE1	-7.01	106.77	120.80
1	A	165	ILE	O-C-N	-7.01	115.50	122.93
1	B	4	THR	CA-C-O	-7.01	112.93	120.92
1	B	3	LYS	O-C-N	7.01	131.49	122.10
1	A	50	LEU	O-C-N	7.01	129.29	122.07
1	C	197	ARG	CD-NE-CZ	-7.00	114.60	124.40
1	A	197	ARG	O-C-N	7.00	130.41	122.22
1	D	100	ILE	O-C-N	7.00	130.48	122.99
1	A	3	LYS	O-C-N	7.00	131.47	122.10
1	B	119	VAL	N-CA-CB	6.99	119.28	110.05
1	C	400	THR	CA-C-O	-6.99	113.75	121.23
1	B	385	ARG	NE-CZ-NH1	6.99	128.49	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	THR	CA-CB-OG1	6.99	120.08	109.60
1	A	89	GLN	OE1-CD-NE2	6.98	129.58	122.60
1	B	384	ALA	N-CA-C	-6.98	103.73	111.82
1	D	235	GLU	N-CA-C	-6.98	103.67	111.28
1	A	361	GLY	O-C-N	6.98	128.88	122.18
1	A	449	VAL	CA-C-O	-6.97	113.19	121.28
1	D	46	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	D	354	ILE	CA-C-N	-6.97	111.13	120.54
1	D	354	ILE	C-N-CA	-6.97	111.13	120.54
1	B	50	LEU	O-C-N	6.97	130.09	122.15
1	B	326	SER	CA-C-O	-6.97	113.16	120.55
1	C	372	PRO	CB-CA-C	-6.96	101.06	110.88
1	A	233	ILE	CA-CB-CG2	6.96	122.33	110.50
1	C	42	GLU	N-CA-CB	6.96	120.16	110.07
1	A	54	MET	CA-C-N	6.95	129.59	120.28
1	A	54	MET	C-N-CA	6.95	129.59	120.28
1	D	50	LEU	O-C-N	6.95	130.07	122.15
1	B	289	ARG	CA-C-O	6.94	126.85	119.50
1	A	225	GLU	CA-C-O	6.93	127.84	120.70
1	B	180	PHE	N-CA-C	-6.93	103.65	111.07
1	D	204	ARG	NH1-CZ-NH2	-6.93	110.29	119.30
1	D	25	ASP	CA-CB-CG	6.93	119.53	112.60
1	D	336	ASP	CA-CB-CG	6.92	119.52	112.60
1	D	278	THR	CA-C-O	-6.92	112.95	121.67
1	B	312	SER	CA-C-O	6.91	122.68	118.33
1	C	177	ASP	CA-CB-CG	6.91	119.50	112.60
1	A	426	THR	CA-C-O	-6.90	113.23	120.55
1	B	149	ASN	CA-C-O	-6.90	113.18	121.05
1	A	436	LEU	CB-CA-C	6.89	122.57	110.85
1	D	30	VAL	CA-C-O	-6.89	113.28	121.28
1	C	250	GLU	N-CA-CB	-6.89	99.69	110.30
1	D	444	HIS	CA-C-O	-6.89	113.80	121.51
1	A	159	ASN	CA-CB-CG	-6.88	105.72	112.60
1	C	70	PRO	CB-CA-C	-6.88	101.14	110.85
1	D	180	PHE	O-C-N	6.88	129.41	122.12
1	B	390	TYR	CA-C-N	-6.88	116.50	123.10
1	B	390	TYR	C-N-CA	-6.88	116.50	123.10
1	C	54	MET	CA-C-N	6.88	130.18	120.28
1	C	54	MET	C-N-CA	6.88	130.18	120.28
1	C	91	PHE	CA-C-N	-6.88	109.68	121.85
1	C	91	PHE	C-N-CA	-6.88	109.68	121.85
1	C	427	ASP	CA-CB-CG	6.87	119.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	258	PHE	N-CA-C	-6.87	103.85	111.82
1	D	437	ALA	CA-C-O	6.87	128.03	120.82
1	A	229	ASN	CA-CB-CG	-6.86	105.74	112.60
1	D	260	GLN	CA-C-O	6.86	128.03	120.82
1	B	392	PRO	CB-CA-C	-6.86	102.61	111.39
1	C	20	LEU	CA-C-N	-6.85	110.56	120.29
1	C	20	LEU	C-N-CA	-6.85	110.56	120.29
1	A	300	ASN	CA-CB-CG	6.85	119.45	112.60
1	D	225	GLU	N-CA-CB	-6.85	100.02	110.16
1	D	295	ALA	O-C-N	6.85	129.38	122.12
1	B	204	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	A	246	ASP	CA-CB-CG	-6.83	105.77	112.60
1	D	206	HIS	CA-CB-CG	-6.82	106.98	113.80
1	D	410	VAL	N-CA-CB	-6.82	101.94	110.47
1	A	289	ARG	CD-NE-CZ	6.82	133.94	124.40
1	C	171	ALA	CB-CA-C	6.82	118.19	109.80
1	A	180	PHE	O-C-N	6.81	129.17	122.09
1	D	210	HIS	N-CA-C	6.80	119.59	110.88
1	B	158	VAL	CA-CB-CG2	-6.80	98.84	110.40
1	B	224	GLN	CG-CD-OE1	6.80	134.40	120.80
1	C	360	ARG	CG-CD-NE	-6.80	97.04	112.00
1	C	401	THR	O-C-N	6.80	130.46	122.24
1	D	449	VAL	N-CA-CB	-6.79	100.30	111.44
1	C	74	THR	N-CA-C	-6.79	101.38	110.55
1	C	180	PHE	CA-CB-CG	6.79	120.58	113.80
1	C	71	GLU	N-CA-C	6.78	119.37	109.07
1	C	90	THR	CB-CA-C	6.77	120.86	109.48
1	A	342	ARG	CB-CG-CD	6.77	126.87	111.30
1	C	423	ILE	CA-C-O	6.77	128.26	121.09
1	A	425	SER	N-CA-C	6.76	118.42	108.14
1	B	322	LEU	O-C-N	-6.76	113.13	122.46
1	A	437	ALA	CA-C-O	6.75	128.13	120.90
1	A	297	ASP	CA-C-O	-6.75	113.73	120.82
1	C	67	THR	OG1-CB-CG2	6.75	122.81	109.30
1	A	355	THR	CA-C-O	6.75	128.12	120.90
1	C	92	THR	CA-C-O	6.75	128.54	120.99
1	C	136	ALA	N-CA-C	6.74	120.28	108.75
1	D	278	THR	CA-CB-CG2	-6.74	99.04	110.50
1	B	227	LEU	CA-C-O	6.74	127.90	120.82
1	D	244	ARG	NE-CZ-NH2	-6.74	113.14	119.20
1	D	369	LEU	CA-C-O	6.74	127.58	119.43
1	C	130	ILE	O-C-N	6.74	130.45	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	411	LEU	CA-C-O	-6.73	111.34	119.49
1	B	257	ILE	N-CA-CB	6.73	122.95	110.77
1	C	183	GLU	OE1-CD-OE2	6.73	139.04	122.90
1	B	108	VAL	CA-CB-CG2	6.73	121.83	110.40
1	B	298	VAL	O-C-N	6.73	128.90	121.90
1	D	277	ALA	CA-C-N	-6.72	110.77	121.86
1	D	277	ALA	C-N-CA	-6.72	110.77	121.86
1	B	257	ILE	O-C-N	6.72	129.39	121.80
1	C	158	VAL	CA-C-O	-6.71	112.81	120.67
1	B	223	ASN	CA-C-O	6.71	128.50	121.38
1	D	110	TYR	CA-C-O	6.71	128.35	120.70
1	A	412	SER	CA-C-O	6.71	128.69	121.05
1	D	218	ILE	O-C-N	6.71	132.62	122.76
1	A	365	THR	O-C-N	6.70	130.94	122.23
1	D	257	ILE	CB-CA-C	-6.70	101.25	112.16
1	D	32	ARG	NE-CZ-NH1	6.69	128.19	121.50
1	B	42	GLU	O-C-N	6.69	128.99	122.03
1	D	68	LYS	O-C-N	6.69	130.93	122.23
1	B	402	ASN	CA-C-O	-6.69	112.94	120.43
1	D	296	GLY	CA-C-O	6.69	127.75	120.66
1	C	302	ILE	N-CA-C	-6.68	103.97	110.72
1	B	460	GLY	O-C-N	-6.68	115.08	122.50
1	C	216	HIS	CG-ND1-CE1	6.68	120.65	109.30
1	A	159	ASN	CB-CG-ND2	-6.67	106.40	116.40
1	A	257	ILE	CB-CA-C	-6.67	101.29	112.16
1	C	173	LYS	CA-C-O	6.67	126.94	119.41
1	C	330	THR	O-C-N	6.67	129.75	122.15
1	B	148	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	C	97	LYS	N-CA-CB	6.65	121.73	110.49
1	D	223	ASN	CA-CB-CG	-6.65	105.95	112.60
1	D	216	HIS	ND1-CG-CD2	-6.65	99.45	106.10
1	A	5	LYS	CA-C-O	6.65	129.34	121.36
1	A	115	THR	N-CA-C	6.64	118.60	111.36
1	C	388	ARG	CB-CG-CD	6.64	126.56	111.30
1	A	89	GLN	CB-CG-CD	-6.63	101.32	112.60
1	D	420	VAL	CA-C-O	-6.63	114.71	121.67
1	C	141	LYS	CA-C-N	-6.63	114.45	123.14
1	C	141	LYS	C-N-CA	-6.63	114.45	123.14
1	A	265	GLU	CA-C-O	-6.63	113.86	120.82
1	C	127	ASP	OD1-CG-OD2	-6.62	107.00	122.90
1	B	268	ILE	O-C-N	6.62	128.40	121.91
1	D	418	GLN	CG-CD-NE2	-6.62	106.48	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	MET	O-C-N	-6.61	114.52	122.65
1	C	245	GLY	O-C-N	-6.61	114.11	122.70
1	A	214	ASN	CA-CB-CG	6.60	119.20	112.60
1	C	390	TYR	CA-C-N	-6.60	116.77	123.10
1	C	390	TYR	C-N-CA	-6.60	116.77	123.10
1	B	412	SER	O-C-N	6.59	130.81	123.16
1	C	257	ILE	N-CA-CB	6.59	123.41	110.95
1	B	156	LYS	CA-CB-CG	-6.59	100.93	114.10
1	A	216	HIS	O-C-N	6.58	131.02	122.93
1	D	231	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	259	ALA	CB-CA-C	6.58	121.29	110.90
1	A	309	VAL	CA-C-N	-6.58	112.08	122.73
1	A	309	VAL	C-N-CA	-6.58	112.08	122.73
1	A	19	MET	N-CA-CB	-6.57	100.55	110.07
1	B	69	GLY	O-C-N	-6.57	115.20	121.77
1	D	29	ASN	CA-CB-CG	-6.57	106.03	112.60
1	B	19	MET	N-CA-CB	-6.56	100.33	109.91
1	D	33	LEU	O-C-N	6.56	131.01	123.27
1	C	453	SER	CB-CA-C	-6.56	98.48	112.78
1	D	60	THR	OG1-CB-CG2	6.56	122.42	109.30
1	A	240	ILE	N-CA-C	6.55	119.54	108.86
1	B	157	GLY	O-C-N	6.55	129.58	122.84
1	A	169	ALA	N-CA-CB	-6.54	100.47	110.16
1	D	285	ILE	N-CA-C	-6.54	102.88	111.05
1	B	15	GLU	CA-C-O	-6.53	110.75	119.11
1	D	52	ASN	OD1-CG-ND2	6.53	129.13	122.60
1	D	404	LYS	CB-CG-CD	6.53	126.31	111.30
1	B	435	GLU	CA-C-O	6.53	127.85	121.00
1	B	397	LEU	CA-C-O	-6.52	113.12	120.43
1	D	309	VAL	CA-C-N	-6.52	112.69	122.74
1	D	309	VAL	C-N-CA	-6.52	112.69	122.74
1	A	158	VAL	N-CA-CB	-6.52	102.41	111.41
1	C	28	MET	CA-CB-CG	-6.52	101.06	114.10
1	D	90	THR	CA-CB-OG1	-6.52	99.82	109.60
1	D	95	THR	CA-CB-OG1	6.52	119.38	109.60
1	D	294	GLU	CA-CB-CG	6.51	127.13	114.10
1	A	53	VAL	O-C-N	6.51	128.19	121.87
1	C	321	PRO	N-CD-CG	-6.51	93.43	103.20
1	B	257	ILE	CB-CA-C	-6.51	101.72	112.26
1	B	396	ILE	CB-CG1-CD1	6.51	127.47	113.80
1	C	360	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	80	GLY	N-CA-C	-6.50	105.07	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLU	N-CA-CB	-6.50	100.58	110.33
1	C	397	LEU	CA-C-O	-6.50	113.78	120.54
1	C	434	LYS	CB-CG-CD	6.50	126.25	111.30
1	A	126	ASP	N-CA-CB	6.50	122.31	111.53
1	C	306	THR	N-CA-C	6.49	119.18	110.35
1	D	141	LYS	N-CA-C	6.49	119.48	108.90
1	A	148	ASN	CA-C-O	6.48	128.01	120.75
1	C	164	SER	O-C-N	6.48	130.61	123.22
1	B	299	ALA	CA-C-O	6.48	127.42	120.55
1	D	257	ILE	O-C-N	6.48	130.69	121.82
1	B	216	HIS	O-C-N	6.47	130.61	123.04
1	C	242	VAL	CB-CA-C	-6.47	103.14	110.96
1	D	410	VAL	CA-C-N	6.47	130.95	120.60
1	D	410	VAL	C-N-CA	6.47	130.95	120.60
1	D	161	PRO	CB-CA-C	-6.46	103.35	111.56
1	A	242	VAL	N-CA-CB	-6.46	103.63	111.00
1	B	300	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	B	377	ALA	CA-C-O	-6.46	113.49	120.92
1	D	235	GLU	CA-C-N	-6.46	110.29	121.66
1	D	235	GLU	C-N-CA	-6.46	110.29	121.66
1	C	450	VAL	CA-C-O	-6.45	113.63	120.53
1	A	324	ALA	CA-C-O	-6.44	114.06	120.70
1	A	356	GLU	CA-C-N	-6.44	111.65	120.28
1	A	356	GLU	C-N-CA	-6.44	111.65	120.28
1	D	80	GLY	N-CA-C	-6.44	105.16	115.08
1	B	86	LYS	CB-CA-C	6.44	121.36	109.70
1	B	404	LYS	O-C-N	6.43	129.48	122.15
1	D	151	ASP	CB-CG-OD2	-6.43	103.61	118.40
1	C	97	LYS	CA-CB-CG	6.43	126.96	114.10
1	B	230	PHE	CA-C-O	6.43	129.70	120.51
1	D	218	ILE	CB-CA-C	-6.42	102.32	111.31
1	C	278	THR	CA-CB-OG1	-6.42	99.97	109.60
1	C	69	GLY	CA-C-N	6.42	126.92	119.99
1	C	69	GLY	C-N-CA	6.42	126.92	119.99
1	A	82	ASP	CA-C-O	-6.41	114.76	121.55
1	B	172	GLU	CB-CG-CD	6.41	123.49	112.60
1	B	91	PHE	CA-CB-CG	6.40	120.20	113.80
1	C	224	GLN	CG-CD-NE2	6.39	125.99	116.40
1	D	425	SER	CA-C-O	-6.39	114.44	121.28
1	C	175	LYS	N-CA-CB	6.39	119.65	110.06
1	C	67	THR	CA-C-O	6.39	129.28	121.99
1	B	99	VAL	CB-CA-C	6.38	120.96	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	MET	CA-C-O	6.38	127.70	121.00
1	C	395	THR	CA-C-O	-6.38	114.14	121.47
1	D	201	ILE	O-C-N	6.38	128.06	121.87
1	A	400	THR	CA-CB-CG2	6.38	121.34	110.50
1	B	95	THR	N-CA-CB	6.38	121.12	110.41
1	C	60	THR	CA-C-O	-6.38	113.91	121.11
1	D	257	ILE	N-CA-CB	6.38	123.00	110.95
1	D	461	THR	CB-CA-C	6.38	121.24	109.70
1	C	172	GLU	CA-C-O	-6.37	111.39	120.51
1	A	249	VAL	CA-C-O	6.37	124.64	119.29
1	B	226	GLY	N-CA-C	-6.37	104.94	112.64
1	C	183	GLU	CG-CD-OE2	-6.37	103.76	118.40
1	D	326	SER	CA-C-O	-6.36	113.81	120.55
1	C	17	GLU	O-C-N	6.36	130.85	122.33
1	C	228	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	A	230	PHE	CA-CB-CG	-6.35	107.45	113.80
1	D	306	THR	N-CA-C	6.35	118.74	110.43
1	C	392	PRO	CB-CA-C	-6.34	103.27	111.39
1	B	42	GLU	N-CA-CB	6.34	119.17	109.91
1	C	149	ASN	CA-CB-CG	6.34	118.94	112.60
1	B	423	ILE	CA-C-O	6.34	128.70	120.78
1	D	166	ALA	N-CA-C	-6.34	105.83	112.93
1	C	92	THR	CA-CB-OG1	-6.33	100.10	109.60
1	B	391	PHE	CA-C-O	-6.33	116.11	120.47
1	A	149	ASN	O-C-N	6.33	130.61	122.89
1	B	231	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	121	ASN	CA-CB-CG	6.32	118.92	112.60
1	C	215	ILE	CA-C-O	-6.32	113.56	120.71
1	C	287	ASN	CA-CB-CG	-6.32	106.28	112.60
1	D	6	ILE	CA-C-N	-6.32	114.90	123.12
1	D	6	ILE	C-N-CA	-6.32	114.90	123.12
1	D	182	CYS	O-C-N	-6.32	115.42	122.12
1	A	300	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	C	114	THR	N-CA-C	6.32	118.24	111.36
1	C	181	GLY	O-C-N	-6.31	116.05	122.17
1	D	156	LYS	O-C-N	6.31	131.00	123.24
1	D	227	LEU	O-C-N	-6.31	115.52	122.09
1	A	405	THR	CB-CA-C	6.31	120.87	110.90
1	A	392	PRO	CB-CA-C	-6.31	103.31	111.39
1	D	227	LEU	CA-C-O	6.31	127.65	120.90
1	A	4	THR	O-C-N	6.30	130.76	122.95
1	D	232	GLU	CA-C-O	-6.30	112.98	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ASN	CB-CA-C	-6.29	98.99	110.63
1	D	177	ASP	CA-C-N	-6.29	110.13	121.14
1	D	177	ASP	C-N-CA	-6.29	110.13	121.14
1	C	124	LEU	O-C-N	6.29	131.20	123.21
1	A	413	LYS	O-C-N	6.29	130.75	122.95
1	B	189	VAL	CA-C-O	-6.29	113.85	120.39
1	D	61	ALA	CA-C-O	-6.29	114.42	121.40
1	C	8	CYS	O-C-N	6.28	130.78	123.30
1	C	129	LEU	CA-C-N	-6.28	114.40	123.06
1	C	129	LEU	C-N-CA	-6.28	114.40	123.06
1	A	268	ILE	CB-CG1-CD1	-6.27	100.64	113.80
1	A	180	PHE	CA-CB-CG	6.27	120.07	113.80
1	C	217	ILE	O-C-N	6.26	130.43	123.10
1	A	133	GLU	CB-CA-C	6.26	120.64	109.38
1	A	151	ASP	CA-C-O	-6.26	113.67	120.36
1	A	76	LYS	N-CA-C	6.25	120.26	110.32
1	B	285	ILE	N-CA-C	-6.25	103.28	111.09
1	D	119	VAL	CA-C-O	-6.25	113.12	120.99
1	A	304	ASP	N-CA-C	-6.25	104.76	112.38
1	D	453	SER	CA-C-O	6.25	127.44	120.94
1	B	438	LEU	O-C-N	6.24	128.83	122.09
1	B	293	ALA	N-CA-CB	6.24	119.42	110.06
1	C	165	ILE	CB-CA-C	-6.24	102.19	110.98
1	D	207	LEU	CA-C-O	6.24	127.03	120.42
1	A	395	THR	CA-CB-OG1	-6.24	100.25	109.60
1	B	78	GLU	O-C-N	6.23	131.61	123.07
1	C	242	VAL	N-CA-CB	-6.23	103.90	111.00
1	A	357	ALA	O-C-N	6.23	128.72	122.12
1	C	48	GLN	CG-CD-NE2	6.23	125.74	116.40
1	C	395	THR	N-CA-CB	6.23	119.75	110.29
1	B	375	VAL	CA-C-N	-6.22	114.47	123.06
1	B	375	VAL	C-N-CA	-6.22	114.47	123.06
1	D	162	GLY	CA-C-O	-6.22	109.75	120.57
1	A	449	VAL	O-C-N	-6.22	116.34	123.00
1	D	356	GLU	O-C-N	6.22	128.56	122.09
1	A	425	SER	CA-C-N	-6.22	111.95	120.28
1	A	425	SER	C-N-CA	-6.22	111.95	120.28
1	A	49	ASN	O-C-N	6.21	128.55	122.09
1	A	140	ASN	CA-C-N	-6.21	112.67	122.73
1	A	140	ASN	C-N-CA	-6.21	112.67	122.73
1	B	235	GLU	CA-C-N	-6.21	110.73	121.66
1	B	235	GLU	C-N-CA	-6.21	110.73	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	VAL	CA-C-O	-6.21	114.43	121.75
1	C	220	LYS	CG-CD-CE	6.20	125.57	111.30
1	D	109	THR	CA-C-N	6.20	132.32	123.14
1	D	109	THR	C-N-CA	6.20	132.32	123.14
1	C	44	GLY	CA-C-N	6.20	129.09	120.29
1	C	44	GLY	C-N-CA	6.20	129.09	120.29
1	D	396	ILE	CB-CG1-CD1	6.19	126.80	113.80
1	D	468	HIS	CA-C-O	-6.19	114.40	121.40
1	B	22	LYS	CA-C-O	-6.19	112.85	119.97
1	C	196	LYS	CB-CG-CD	6.19	125.53	111.30
1	B	275	ILE	CB-CG1-CD1	6.17	126.76	113.80
1	D	105	MET	N-CA-CB	-6.17	102.18	111.56
1	A	447	ASP	CA-C-O	6.17	128.76	121.36
1	B	133	GLU	CA-C-N	-6.17	114.66	122.37
1	B	133	GLU	C-N-CA	-6.17	114.66	122.37
1	C	73	ARG	N-CA-C	6.17	120.10	110.17
1	C	188	PHE	CA-C-O	-6.16	114.44	121.40
1	D	70	PRO	CA-C-O	-6.16	114.48	122.12
1	B	1	MET	CB-CG-SD	6.16	131.18	112.70
1	B	405	THR	CB-CA-C	6.16	121.32	110.85
1	C	107	ALA	N-CA-CB	-6.16	100.26	110.23
1	C	130	ILE	CA-C-O	-6.16	113.47	120.67
1	C	25	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	193	PHE	O-C-N	-6.14	115.30	122.86
1	B	29	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	D	453	SER	N-CA-CB	-6.14	101.95	111.35
1	B	165	ILE	N-CA-CB	-6.14	99.85	111.21
1	D	200	VAL	N-CA-C	6.14	116.88	110.62
1	D	51	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	D	198	SER	CA-C-O	6.14	127.26	120.63
1	D	208	LYS	N-CA-C	-6.14	104.67	111.36
1	A	289	ARG	O-C-N	6.13	128.38	121.94
1	B	108	VAL	CA-C-O	6.13	129.42	121.32
1	A	103	SER	CA-C-N	-6.13	112.62	122.24
1	A	103	SER	C-N-CA	-6.13	112.62	122.24
1	B	387	VAL	N-CA-C	-6.12	103.71	112.35
1	C	342	ARG	CA-C-O	-6.12	112.86	120.57
1	B	123	VAL	CA-CB-CG2	-6.11	100.01	110.40
1	B	385	ARG	NH1-CZ-NH2	6.11	127.24	119.30
1	A	192	SER	N-CA-C	6.11	118.80	110.55
1	A	2	LYS	N-CA-CB	6.11	118.60	110.29
1	C	82	ASP	CA-CB-CG	6.11	118.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	GLU	CA-C-N	-6.11	113.16	119.94
1	C	225	GLU	C-N-CA	-6.11	113.16	119.94
1	C	452	VAL	CA-C-O	-6.11	113.53	120.67
1	C	57	THR	CB-CA-C	-6.10	98.77	109.02
1	D	291	THR	O-C-N	6.10	129.92	123.03
1	C	337	ARG	NH1-CZ-NH2	6.10	127.23	119.30
1	C	449	VAL	CA-C-O	-6.09	113.84	120.67
1	D	263	MET	CA-CB-CG	6.09	126.29	114.10
1	D	317	LYS	O-C-N	6.09	128.47	122.19
1	B	356	GLU	CA-C-O	-6.09	114.09	120.55
1	C	192	SER	N-CA-C	6.09	119.50	110.48
1	B	124	LEU	N-CA-C	-6.09	99.98	109.72
1	B	436	LEU	N-CA-CB	-6.09	100.93	110.06
1	C	168	PRO	N-CA-CB	6.09	111.46	103.42
1	C	190	ALA	O-C-N	6.09	130.16	123.22
1	D	244	ARG	CD-NE-CZ	6.09	132.92	124.40
1	C	46	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	A	302	ILE	N-CA-CB	6.08	117.67	110.55
1	B	314	GLU	CA-C-O	-6.08	113.23	120.10
1	B	165	ILE	CA-C-O	6.08	127.64	120.72
1	A	49	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	C	385	ARG	CG-CD-NE	-6.07	98.64	112.00
1	A	402	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	B	294	GLU	CA-CB-CG	6.07	126.24	114.10
1	C	231	ASP	CA-C-N	-6.06	110.60	120.72
1	C	231	ASP	C-N-CA	-6.06	110.60	120.72
1	A	325	VAL	CA-C-O	6.06	127.57	121.27
1	A	16	SER	CA-C-O	6.06	128.53	121.87
1	B	50	LEU	N-CA-C	-6.06	104.76	111.36
1	B	60	THR	OG1-CB-CG2	6.06	121.41	109.30
1	C	362	ALA	CA-C-O	6.06	126.97	120.55
1	D	275	ILE	O-C-N	6.05	129.80	123.26
1	D	74	THR	N-CA-C	-6.05	101.56	110.52
1	B	164	SER	CB-CA-C	-6.05	100.36	110.29
1	B	174	ASP	CB-CG-OD1	6.05	132.32	118.40
1	B	228	ASN	O-C-N	-6.04	115.15	122.22
1	C	50	LEU	CA-C-N	-6.04	111.58	120.28
1	C	50	LEU	C-N-CA	-6.04	111.58	120.28
1	D	170	LEU	N-CA-C	6.04	118.48	108.99
1	A	43	HIS	ND1-CG-CD2	-6.04	100.06	106.10
1	D	135	THR	CA-CB-CG2	-6.04	100.23	110.50
1	A	309	VAL	CA-C-O	-6.04	113.61	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	GLU	CA-CB-CG	-6.04	102.03	114.10
1	C	60	THR	CA-C-N	-6.04	112.52	122.11
1	C	60	THR	C-N-CA	-6.04	112.52	122.11
1	D	413	LYS	CB-CG-CD	6.03	125.18	111.30
1	A	439	GLN	N-CA-CB	6.03	119.51	110.22
1	C	239	GLY	CA-C-O	6.03	127.90	121.75
1	D	38	GLY	O-C-N	-6.03	116.27	122.60
1	A	297	ASP	N-CA-C	-6.03	104.62	111.07
1	B	47	ILE	O-C-N	6.03	127.72	121.87
1	A	26	ALA	O-C-N	6.02	131.22	122.43
1	B	330	THR	N-CA-CB	6.02	119.07	110.16
1	A	1	MET	CB-CG-SD	6.01	130.74	112.70
1	D	262	MET	CA-C-N	-6.01	111.75	120.29
1	D	262	MET	C-N-CA	-6.01	111.75	120.29
1	D	10	ILE	CA-C-O	6.01	127.14	120.59
1	D	232	GLU	CB-CA-C	6.01	121.75	110.63
1	B	28	MET	CA-C-O	-6.00	115.19	121.55
1	D	278	THR	N-CA-CB	-6.00	101.81	110.45
1	D	143	ILE	CB-CG1-CD1	-6.00	101.20	113.80
1	A	356	GLU	CB-CG-CD	6.00	122.80	112.60
1	C	4	THR	CA-C-O	-6.00	114.59	121.19
1	A	340	ASN	OD1-CG-ND2	6.00	128.59	122.60
1	C	173	LYS	CA-C-N	-5.99	112.65	120.44
1	C	173	LYS	C-N-CA	-5.99	112.65	120.44
1	A	224	GLN	CB-CG-CD	5.99	122.78	112.60
1	A	321	PRO	N-CD-CG	-5.99	94.21	103.20
1	B	434	LYS	CB-CG-CD	5.98	125.05	111.30
1	B	120	GLY	CA-C-O	5.98	125.31	119.27
1	C	413	LYS	O-C-N	5.97	130.36	122.95
1	C	452	VAL	CB-CA-C	-5.97	101.72	110.62
1	D	245	GLY	CA-C-N	5.97	128.56	120.38
1	D	245	GLY	C-N-CA	5.97	128.56	120.38
1	C	194	ILE	CA-CB-CG1	-5.97	100.25	110.40
1	B	409	LEU	CA-C-O	5.96	126.71	119.49
1	D	235	GLU	CB-CG-CD	5.96	122.73	112.60
1	D	389	LYS	CA-C-O	-5.96	114.19	120.63
1	B	233	ILE	CA-C-O	5.96	127.66	121.05
1	B	287	ASN	CB-CG-ND2	5.96	125.33	116.40
1	C	31	MET	O-C-N	-5.96	116.28	123.13
1	A	276	THR	CA-C-O	5.95	126.73	120.36
1	B	130	ILE	CA-C-O	-5.95	113.71	120.67
1	B	43	HIS	CG-CD2-NE2	5.95	113.15	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	VAL	N-CA-CB	-5.95	101.69	111.44
1	A	413	LYS	N-CA-CB	5.95	118.79	109.69
1	B	167	LEU	CB-CA-C	-5.95	99.71	109.46
1	C	81	ASN	O-C-N	5.95	130.15	123.19
1	C	289	ARG	CA-C-O	-5.95	113.85	119.91
1	B	108	VAL	O-C-N	-5.94	116.79	123.03
1	A	287	ASN	CA-CB-CG	-5.94	106.66	112.60
1	D	292	ARG	CD-NE-CZ	5.94	132.72	124.40
1	B	468	HIS	CA-C-N	-5.94	115.45	122.93
1	B	468	HIS	C-N-CA	-5.94	115.45	122.93
1	A	116	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	232	GLU	CA-C-O	-5.94	112.31	119.49
1	D	296	GLY	O-C-N	-5.94	116.43	122.19
1	A	193	PHE	CA-C-O	5.93	129.16	122.27
1	D	434	LYS	CB-CG-CD	5.93	124.94	111.30
1	C	216	HIS	N-CA-CB	5.93	119.01	110.06
1	A	71	GLU	CA-CB-CG	5.93	125.96	114.10
1	C	43	HIS	ND1-CE1-NE2	-5.93	102.47	108.40
1	C	171	ALA	O-C-N	-5.92	115.54	122.89
1	A	375	VAL	N-CA-CB	-5.92	103.20	111.25
1	B	185	GLY	CA-C-O	-5.92	113.07	119.82
1	C	163	VAL	N-CA-C	5.92	117.26	109.21
1	B	321	PRO	N-CD-CG	-5.92	94.32	103.20
1	D	365	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	110	TYR	N-CA-C	5.91	119.36	107.41
1	A	292	ARG	CD-NE-CZ	5.91	132.68	124.40
1	D	144	CYS	N-CA-CB	-5.91	101.88	111.22
1	A	304	ASP	CA-C-O	-5.91	112.34	119.49
1	A	224	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	354	ILE	CA-C-N	-5.90	112.58	120.54
1	A	354	ILE	C-N-CA	-5.90	112.58	120.54
1	A	390	TYR	CA-CB-CG	-5.90	103.28	113.90
1	D	7	VAL	CA-C-O	-5.90	114.22	120.53
1	A	141	LYS	CB-CG-CD	5.90	124.86	111.30
1	B	143	ILE	CA-CB-CG2	5.89	120.52	110.50
1	C	268	ILE	CA-C-O	-5.89	114.60	120.85
1	A	275	ILE	O-C-N	5.89	129.54	123.18
1	B	133	GLU	O-C-N	5.89	130.69	123.21
1	D	402	ASN	N-CA-CB	-5.89	100.27	110.17
1	C	439	GLN	O-C-N	5.89	128.92	122.20
1	B	427	ASP	OD1-CG-OD2	-5.89	108.77	122.90
1	D	178	LEU	N-CA-CB	-5.89	100.80	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	LYS	N-CA-CB	5.89	119.07	110.47
1	A	213	GLU	N-CA-C	5.89	119.56	112.38
1	C	279	MET	N-CA-C	5.89	119.55	111.54
1	D	104	GLU	CB-CG-CD	5.89	122.61	112.60
1	B	89	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	158	VAL	CA-C-O	-5.88	114.22	120.39
1	B	29	ASN	CA-C-N	-5.88	114.25	122.71
1	B	29	ASN	C-N-CA	-5.88	114.25	122.71
1	D	28	MET	CA-CB-CG	-5.88	102.34	114.10
1	A	418	GLN	CG-CD-OE1	5.88	132.55	120.80
1	D	240	ILE	N-CA-C	5.87	118.65	108.90
1	B	427	ASP	CB-CG-OD1	5.87	131.90	118.40
1	A	184	GLN	CA-C-N	-5.87	111.41	120.91
1	A	184	GLN	C-N-CA	-5.87	111.41	120.91
1	B	195	ARG	CG-CD-NE	5.87	124.91	112.00
1	C	166	ALA	CA-C-N	-5.87	112.16	120.49
1	C	166	ALA	C-N-CA	-5.87	112.16	120.49
1	D	423	ILE	CA-C-O	5.87	126.67	120.51
1	B	367	GLU	CA-C-O	5.86	126.64	120.42
1	B	114	THR	CA-CB-OG1	-5.86	100.81	109.60
1	C	163	VAL	CA-C-O	-5.86	114.14	121.11
1	B	238	ASP	O-C-N	5.86	129.66	122.34
1	D	66	ASP	N-CA-C	5.86	117.84	108.41
1	B	67	THR	N-CA-CB	5.85	118.73	110.36
1	A	238	ASP	N-CA-C	-5.85	105.80	113.17
1	A	314	GLU	O-C-N	5.85	129.06	122.22
1	B	162	GLY	CA-C-O	-5.85	110.39	120.57
1	D	311	LEU	N-CA-CB	5.85	119.71	110.23
1	A	210	HIS	ND1-CE1-NE2	-5.85	102.55	108.40
1	C	337	ARG	CA-C-N	-5.84	111.45	121.97
1	C	337	ARG	C-N-CA	-5.84	111.45	121.97
1	A	282	ASP	CA-CB-CG	5.84	118.44	112.60
1	D	449	VAL	O-C-N	-5.83	116.86	123.10
1	D	214	ASN	CA-CB-CG	5.83	118.43	112.60
1	B	155	ASN	CB-CG-OD1	-5.83	109.14	120.80
1	D	388	ARG	CA-CB-CG	5.83	125.76	114.10
1	D	11	GLY	CA-C-O	5.83	129.85	121.52
1	A	203	ILE	CA-C-O	5.82	126.76	120.47
1	C	44	GLY	N-CA-C	5.82	119.72	112.73
1	C	193	PHE	CA-C-O	5.82	129.36	122.14
1	A	331	ILE	CB-CA-C	-5.82	104.28	112.14
1	A	115	THR	CA-CB-CG2	-5.82	100.60	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	ILE	CB-CG1-CD1	-5.82	101.58	113.80
1	B	136	ALA	N-CA-C	5.82	117.95	108.76
1	B	227	LEU	O-C-N	-5.82	116.08	122.07
1	B	264	ILE	CA-C-O	5.82	127.33	121.17
1	B	379	GLN	OE1-CD-NE2	5.82	128.42	122.60
1	A	154	GLU	CB-CA-C	-5.81	99.94	109.53
1	C	216	HIS	ND1-CE1-NE2	-5.81	102.59	108.40
1	B	51	ARG	N-CA-C	-5.81	105.45	112.54
1	C	246	ASP	CB-CG-OD1	5.81	131.77	118.40
1	C	184	GLN	N-CA-C	-5.81	105.69	112.89
1	D	280	MET	CG-SD-CE	5.81	113.68	100.90
1	A	159	ASN	CA-C-O	-5.81	114.60	121.16
1	C	32	ARG	CD-NE-CZ	5.81	132.53	124.40
1	C	437	ALA	O-C-N	-5.81	116.09	122.07
1	C	290	PRO	N-CA-C	-5.81	100.51	112.47
1	A	163	VAL	N-CA-C	5.80	117.10	109.21
1	A	439	GLN	CA-C-O	-5.80	113.54	120.10
1	C	210	HIS	ND1-CG-CD2	-5.80	100.30	106.10
1	B	195	ARG	CA-C-N	-5.80	111.01	121.62
1	B	195	ARG	C-N-CA	-5.80	111.01	121.62
1	D	334	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	A	306	THR	N-CA-C	5.79	118.01	110.43
1	B	372	PRO	CB-CA-C	-5.79	102.30	111.04
1	C	336	ASP	N-CA-C	-5.79	104.97	111.28
1	A	253	VAL	N-CA-C	5.79	116.44	110.36
1	B	328	MET	CA-C-O	5.79	126.68	120.55
1	B	356	GLU	CB-CA-C	-5.78	101.20	110.79
1	A	254	GLU	CA-C-O	-5.78	111.82	119.10
1	A	50	LEU	CA-C-N	-5.78	112.54	120.28
1	A	50	LEU	C-N-CA	-5.78	112.54	120.28
1	A	197	ARG	CA-C-O	-5.78	113.57	120.10
1	D	48	GLN	OE1-CD-NE2	5.77	128.37	122.60
1	C	294	GLU	O-C-N	-5.77	116.12	122.07
1	A	74	THR	CA-C-N	-5.77	116.81	123.04
1	A	74	THR	C-N-CA	-5.77	116.81	123.04
1	B	150	GLY	CA-C-N	-5.77	115.04	123.00
1	B	150	GLY	C-N-CA	-5.77	115.04	123.00
1	D	88	GLY	CA-C-O	5.77	125.78	119.55
1	D	443	ALA	CA-C-O	-5.77	115.28	121.45
1	B	150	GLY	CA-C-O	-5.77	115.97	121.62
1	B	320	TYR	CB-CG-CD1	-5.77	112.15	120.80
1	C	354	ILE	N-CA-CB	5.77	121.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ALA	CA-C-O	-5.77	112.85	119.60
1	D	29	ASN	CA-C-N	-5.76	113.52	122.69
1	D	29	ASN	C-N-CA	-5.76	113.52	122.69
1	C	1	MET	CB-CG-SD	5.76	129.99	112.70
1	C	238	ASP	O-C-N	5.76	129.96	122.42
1	C	324	ALA	CA-C-N	-5.76	113.17	120.60
1	C	324	ALA	C-N-CA	-5.76	113.17	120.60
1	A	423	ILE	CA-C-O	5.76	126.56	120.51
1	A	11	GLY	CA-C-N	5.75	125.29	119.19
1	A	11	GLY	C-N-CA	5.75	125.29	119.19
1	A	146	VAL	CA-C-N	-5.75	113.45	122.65
1	A	146	VAL	C-N-CA	-5.75	113.45	122.65
1	A	177	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	160	LEU	O-C-N	5.75	126.46	121.34
1	B	316	ALA	N-CA-C	-5.75	105.93	113.12
1	C	164	SER	CA-C-O	-5.75	114.04	120.54
1	D	60	THR	CB-CA-C	-5.75	98.01	109.33
1	C	30	VAL	CB-CA-C	-5.74	100.78	110.71
1	C	257	ILE	CB-CA-C	-5.73	102.81	112.16
1	C	60	THR	CB-CA-C	-5.73	98.03	109.33
1	D	105	MET	CG-SD-CE	5.73	113.51	100.90
1	D	265	GLU	CA-CB-CG	5.73	125.56	114.10
1	C	373	LEU	O-C-N	5.72	130.01	123.48
1	C	356	GLU	CB-CA-C	-5.72	101.66	110.81
1	A	269	ARG	O-C-N	-5.72	115.53	122.22
1	C	47	ILE	O-C-N	5.72	127.72	121.83
1	A	17	GLU	O-C-N	5.71	128.17	122.12
1	B	111	GLU	N-CA-CB	-5.71	101.12	110.14
1	C	259	ALA	CB-CA-C	5.71	119.92	110.90
1	D	46	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	D	292	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	D	324	ALA	N-CA-CB	5.70	118.34	110.07
1	D	451	MET	CA-C-O	-5.70	114.17	120.38
1	A	168	PRO	CA-C-N	5.70	128.38	120.29
1	A	168	PRO	C-N-CA	5.70	128.38	120.29
1	A	314	GLU	N-CA-C	-5.70	105.16	111.71
1	A	416	VAL	O-C-N	5.70	126.43	120.96
1	B	356	GLU	O-C-N	5.69	128.16	122.12
1	C	241	MET	CA-C-N	5.69	129.49	122.37
1	C	241	MET	C-N-CA	5.69	129.49	122.37
1	C	340	ASN	N-CA-C	5.69	118.83	109.72
1	A	393	ASP	CA-CB-CG	-5.69	106.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LYS	N-CA-CB	-5.69	100.96	110.80
1	B	322	LEU	N-CA-CB	-5.69	101.13	110.40
1	C	339	MET	CA-C-O	-5.69	114.72	121.66
1	B	235	GLU	CB-CG-CD	5.68	122.26	112.60
1	C	287	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	B	36	SER	N-CA-C	-5.68	105.62	112.54
1	C	189	VAL	CA-C-O	-5.68	114.48	120.39
1	A	184	GLN	CA-C-O	-5.67	112.27	119.31
1	C	4	THR	N-CA-C	-5.67	102.00	110.23
1	B	422	GLU	CB-CG-CD	5.67	122.24	112.60
1	C	330	THR	CA-C-O	-5.67	114.41	120.42
1	D	238	ASP	CA-C-O	-5.67	112.71	119.35
1	D	190	ALA	CA-C-N	-5.67	114.64	122.30
1	D	190	ALA	C-N-CA	-5.67	114.64	122.30
1	A	372	PRO	O-C-N	5.67	130.13	122.37
1	D	377	ALA	CA-C-O	-5.67	114.51	120.80
1	A	216	HIS	CG-ND1-CE1	5.66	118.93	109.30
1	A	39	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	213	GLU	CA-C-O	-5.66	112.93	119.61
1	A	423	ILE	CB-CA-C	5.66	117.37	111.09
1	B	391	PHE	O-C-N	5.66	127.82	121.32
1	D	66	ASP	O-C-N	5.65	129.71	122.93
1	A	200	VAL	N-CA-C	5.65	116.29	110.36
1	D	363	VAL	CA-C-O	5.65	126.75	120.71
1	D	172	GLU	CA-C-N	-5.64	112.15	120.28
1	D	172	GLU	C-N-CA	-5.64	112.15	120.28
1	D	331	ILE	CA-C-O	-5.64	114.78	121.05
1	A	197	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	B	391	PHE	CA-CB-CG	-5.64	108.16	113.80
1	D	123	VAL	N-CA-CB	-5.64	103.62	111.41
1	C	329	ALA	CA-C-O	-5.64	113.98	120.24
1	D	438	LEU	O-C-N	5.64	128.18	122.09
1	B	309	VAL	CA-C-O	-5.64	113.88	121.32
1	B	382	LYS	CA-C-N	-5.64	111.10	120.68
1	B	382	LYS	C-N-CA	-5.64	111.10	120.68
1	D	127	ASP	CB-CA-C	-5.64	103.21	112.06
1	B	201	ILE	CA-C-N	-5.63	112.29	120.29
1	B	201	ILE	C-N-CA	-5.63	112.29	120.29
1	D	32	ARG	NH1-CZ-NH2	-5.63	111.98	119.30
1	C	385	ARG	CA-C-O	5.63	126.43	119.79
1	B	16	SER	O-C-N	-5.63	116.38	122.79
1	C	186	VAL	CA-CB-CG1	-5.63	100.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	VAL	O-C-N	5.63	129.02	123.00
1	D	4	THR	CA-CB-CG2	5.62	120.06	110.50
1	A	228	ASN	CA-C-O	-5.62	114.92	120.82
1	B	292	ARG	CD-NE-CZ	5.62	132.27	124.40
1	D	213	GLU	CA-CB-CG	-5.62	102.86	114.10
1	D	27	GLY	O-C-N	-5.62	115.40	122.70
1	B	172	GLU	OE1-CD-OE2	-5.62	109.42	122.90
1	B	40	TYR	CA-C-O	-5.61	113.76	120.10
1	A	388	ARG	CG-CD-NE	5.61	124.34	112.00
1	C	375	VAL	CB-CA-C	5.61	119.19	110.83
1	A	223	ASN	CA-C-O	5.61	127.31	121.36
1	B	176	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	C	129	LEU	O-C-N	5.61	128.98	122.20
1	D	343	LEU	CA-C-O	5.61	127.32	120.31
1	B	178	LEU	CA-C-O	-5.61	113.52	119.97
1	C	275	ILE	CA-C-N	-5.61	115.31	122.77
1	C	275	ILE	C-N-CA	-5.61	115.31	122.77
1	D	216	HIS	CB-CG-CD2	5.60	138.48	131.20
1	D	360	ARG	N-CA-C	-5.60	105.26	111.36
1	B	206	HIS	CB-CA-C	5.59	120.94	110.70
1	C	328	MET	CB-CA-C	-5.59	101.17	110.68
1	D	87	ALA	CA-C-O	-5.59	115.00	121.15
1	D	113	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	261	LYS	CB-CG-CD	5.59	124.16	111.30
1	D	392	PRO	CB-CA-C	-5.59	104.23	111.39
1	A	154	GLU	CB-CG-CD	5.59	122.10	112.60
1	B	68	LYS	CA-C-O	-5.59	114.57	120.55
1	A	187	ASP	O-C-N	-5.59	114.81	122.46
1	B	287	ASN	O-C-N	5.58	126.10	121.35
1	A	79	GLY	O-C-N	5.58	129.96	122.70
1	A	434	LYS	CB-CA-C	5.58	119.72	110.90
1	B	469	VAL	O-C-N	5.58	129.22	123.03
1	D	329	ALA	CA-C-N	-5.58	112.37	120.29
1	D	329	ALA	C-N-CA	-5.58	112.37	120.29
1	A	210	HIS	CA-CB-CG	-5.58	108.22	113.80
1	B	8	CYS	N-CA-C	5.58	118.05	109.07
1	D	151	ASP	CA-C-O	5.58	126.62	120.71
1	D	342	ARG	CA-C-O	-5.57	113.55	120.57
1	B	235	GLU	N-CA-C	-5.57	105.21	111.28
1	C	72	ILE	CB-CA-C	-5.56	104.92	111.09
1	D	320	TYR	CA-CB-CG	-5.56	103.89	113.90
1	A	257	ILE	CB-CG1-CD1	-5.56	102.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	MET	N-CA-C	5.56	122.64	110.80
1	B	222	GLU	N-CA-CB	-5.56	102.95	110.95
1	B	263	MET	CA-CB-CG	5.56	125.22	114.10
1	D	173	LYS	CA-C-N	5.56	128.50	120.38
1	D	173	LYS	C-N-CA	5.56	128.50	120.38
1	B	146	VAL	CA-CB-CG2	-5.55	100.96	110.40
1	D	74	THR	CA-C-N	-5.55	117.19	123.13
1	D	74	THR	C-N-CA	-5.55	117.19	123.13
1	D	21	ALA	CA-C-N	5.55	128.17	120.29
1	D	21	ALA	C-N-CA	5.55	128.17	120.29
1	D	357	ALA	CA-C-O	-5.55	115.00	120.82
1	C	136	ALA	CB-CA-C	-5.54	98.70	109.68
1	C	455	ALA	CB-CA-C	5.54	119.73	109.70
1	A	205	GLU	CA-C-O	5.54	126.39	120.24
1	A	361	GLY	N-CA-C	-5.54	106.08	112.50
1	A	431	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	D	409	LEU	O-C-N	-5.54	115.01	122.43
1	D	40	TYR	CA-C-O	-5.53	114.65	120.63
1	C	454	GLY	CA-C-N	-5.53	114.22	122.74
1	C	454	GLY	C-N-CA	-5.53	114.22	122.74
1	A	457	VAL	N-CA-CB	5.53	118.95	111.21
1	A	36	SER	N-CA-C	-5.53	105.64	112.38
1	B	225	GLU	CA-C-O	5.52	126.62	120.82
1	C	323	GLU	N-CA-C	-5.52	104.90	111.69
1	C	200	VAL	N-CA-C	5.52	116.91	110.62
1	A	179	ILE	CA-CB-CG1	-5.52	101.02	110.40
1	B	217	ILE	CB-CA-C	-5.52	103.33	110.84
1	B	80	GLY	N-CA-C	-5.52	106.40	114.90
1	B	156	LYS	O-C-N	5.52	130.03	123.24
1	B	400	THR	O-C-N	5.52	129.66	123.48
1	D	197	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	D	340	ASN	CA-C-O	-5.52	115.17	121.40
1	B	415	VAL	CB-CA-C	-5.51	103.20	110.98
1	A	356	GLU	CA-CB-CG	5.51	125.13	114.10
1	A	53	VAL	CA-C-N	-5.51	113.38	120.65
1	A	53	VAL	C-N-CA	-5.51	113.38	120.65
1	C	462	THR	CA-C-N	-5.51	113.32	122.08
1	C	462	THR	C-N-CA	-5.51	113.32	122.08
1	A	278	THR	CA-CB-CG2	-5.50	101.14	110.50
1	C	253	VAL	CB-CA-C	-5.50	102.27	111.29
1	C	265	GLU	CA-C-O	-5.50	114.72	120.55
1	D	372	PRO	CB-CA-C	-5.50	102.74	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ILE	CA-C-O	5.50	127.12	120.85
1	A	70	PRO	N-CA-C	5.49	119.70	111.14
1	D	68	LYS	CA-C-O	-5.49	114.14	120.24
1	B	416	VAL	O-C-N	-5.49	117.91	121.37
1	C	32	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	D	322	LEU	O-C-N	-5.49	115.52	122.27
1	A	119	VAL	CA-C-O	-5.49	114.08	120.99
1	B	85	LEU	CB-CA-C	5.49	118.89	109.51
1	C	84	SER	CB-CA-C	5.48	119.37	110.22
1	A	32	ARG	CD-NE-CZ	5.48	132.07	124.40
1	B	293	ALA	O-C-N	5.48	127.92	122.12
1	B	222	GLU	CG-CD-OE1	5.47	130.99	118.40
1	B	431	ARG	CA-C-N	5.47	127.87	120.65
1	B	431	ARG	C-N-CA	5.47	127.87	120.65
1	B	143	ILE	CA-C-N	-5.47	113.27	123.01
1	B	143	ILE	C-N-CA	-5.47	113.27	123.01
1	C	53	VAL	O-C-N	5.47	127.18	121.87
1	C	360	ARG	O-C-N	5.47	127.92	122.12
1	B	452	VAL	CB-CA-C	-5.47	102.40	110.82
1	D	427	ASP	OD1-CG-OD2	-5.47	109.78	122.90
1	B	110	TYR	CA-C-O	5.47	126.93	120.70
1	A	154	GLU	OE1-CD-OE2	-5.46	109.78	122.90
1	B	190	ALA	CA-C-O	-5.46	114.51	120.36
1	B	363	VAL	CA-C-N	-5.46	112.96	120.28
1	B	363	VAL	C-N-CA	-5.46	112.96	120.28
1	A	84	SER	CA-C-O	-5.46	114.74	120.58
1	B	278	THR	CA-CB-OG1	-5.46	101.41	109.60
1	B	135	THR	O-C-N	5.46	130.11	122.36
1	A	204	ARG	CA-C-O	5.45	126.24	119.97
1	D	99	VAL	O-C-N	5.45	128.24	122.62
1	D	384	ALA	N-CA-C	-5.45	105.49	111.82
1	A	375	VAL	CA-C-O	5.45	126.26	120.48
1	D	110	TYR	N-CA-C	5.45	118.35	107.62
1	A	360	ARG	CG-CD-NE	-5.45	100.02	112.00
1	C	217	ILE	CB-CA-C	-5.45	103.01	110.96
1	B	51	ARG	CD-NE-CZ	5.44	132.02	124.40
1	B	10	ILE	CA-C-O	5.44	126.39	120.57
1	A	45	GLN	N-CA-C	-5.44	105.43	111.36
1	D	155	ASN	N-CA-CB	-5.43	101.31	110.49
1	D	49	ASN	CB-CG-OD1	5.43	131.66	120.80
1	D	217	ILE	O-C-N	5.43	129.45	123.10
1	D	169	ALA	CA-C-O	5.43	126.28	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	THR	N-CA-C	-5.43	105.44	111.36
1	B	451	MET	CA-C-O	-5.42	114.47	120.38
1	C	340	ASN	CA-C-O	-5.42	114.98	121.11
1	A	66	ASP	O-C-N	5.42	129.40	123.22
1	A	372	PRO	CB-CA-C	-5.42	102.85	111.04
1	B	314	GLU	N-CA-C	-5.42	105.47	111.71
1	B	357	ALA	N-CA-C	-5.42	105.28	111.14
1	C	129	LEU	CB-CA-C	-5.42	101.84	110.84
1	D	165	ILE	CA-CB-CG1	-5.42	101.18	110.40
1	D	175	LYS	CA-C-O	-5.42	114.22	120.24
1	D	374	ILE	O-C-N	-5.42	117.41	123.26
1	D	436	LEU	N-CA-CB	-5.42	101.94	110.06
1	B	314	GLU	CA-C-N	-5.42	113.73	122.23
1	B	314	GLU	C-N-CA	-5.42	113.73	122.23
1	A	176	GLN	CB-CG-CD	5.41	121.80	112.60
1	A	307	ASP	N-CA-C	-5.41	104.92	112.45
1	C	202	GLU	CA-C-O	5.41	126.19	119.97
1	B	425	SER	CA-C-O	-5.41	115.49	121.28
1	B	170	LEU	N-CA-C	5.41	118.37	109.72
1	C	356	GLU	CB-CG-CD	5.41	121.79	112.60
1	C	391	PHE	CA-C-O	5.41	124.20	120.47
1	A	279	MET	N-CA-C	5.41	118.89	111.54
1	C	341	SER	CA-C-O	-5.41	115.92	121.87
1	D	73	ARG	CG-CD-NE	5.41	123.89	112.00
1	D	35	PHE	N-CA-C	-5.40	106.54	113.02
1	C	70	PRO	N-CA-C	5.40	120.55	111.32
1	C	402	ASN	N-CA-CB	-5.40	101.62	110.42
1	A	302	ILE	N-CA-C	-5.40	105.24	110.42
1	C	167	LEU	CB-CA-C	5.40	117.90	109.42
1	C	398	ALA	CB-CA-C	-5.40	101.33	110.19
1	C	455	ALA	CA-C-O	-5.39	114.33	120.32
1	D	169	ALA	N-CA-CB	-5.39	101.63	110.14
1	A	74	THR	CA-CB-CG2	5.39	119.66	110.50
1	A	93	PHE	CA-CB-CG	5.39	119.19	113.80
1	D	230	PHE	CA-C-N	5.38	127.76	120.65
1	D	230	PHE	C-N-CA	5.38	127.76	120.65
1	B	331	ILE	N-CA-CB	5.38	116.85	110.55
1	B	213	GLU	CA-CB-CG	-5.38	103.34	114.10
1	C	171	ALA	N-CA-CB	-5.38	100.90	109.19
1	D	64	LEU	O-C-N	-5.38	116.02	123.12
1	A	28	MET	CA-CB-CG	-5.38	103.34	114.10
1	A	78	GLU	CA-CB-CG	-5.38	103.35	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	462	THR	O-C-N	5.38	129.51	123.27
1	D	289	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	343	LEU	CA-C-O	5.37	127.03	120.31
1	D	393	ASP	N-CA-C	-5.37	105.46	112.23
1	D	255	GLU	CA-CB-CG	-5.37	103.36	114.10
1	A	197	ARG	NH1-CZ-NH2	5.37	126.28	119.30
1	B	328	MET	O-C-N	-5.37	116.43	122.12
1	D	313	GLY	O-C-N	5.37	129.67	122.70
1	B	197	ARG	N-CA-CB	-5.36	102.02	110.06
1	D	24	LEU	N-CA-C	-5.36	104.68	111.11
1	A	235	GLU	CB-CG-CD	5.36	121.71	112.60
1	C	143	ILE	CA-CB-CG1	-5.35	101.30	110.40
1	B	388	ARG	CA-CB-CG	5.35	124.80	114.10
1	D	275	ILE	CA-C-O	-5.35	114.77	120.39
1	C	74	THR	CA-C-O	-5.35	115.50	121.81
1	D	284	MET	N-CA-C	-5.35	106.83	113.19
1	D	145	LYS	CG-CD-CE	5.34	123.59	111.30
1	D	212	GLY	CA-C-N	5.34	129.23	120.63
1	D	212	GLY	C-N-CA	5.34	129.23	120.63
1	C	159	ASN	CB-CA-C	5.34	119.57	109.37
1	D	54	MET	CG-SD-CE	-5.34	89.15	100.90
1	D	149	ASN	O-C-N	5.34	129.41	122.89
1	D	326	SER	N-CA-C	5.34	117.10	111.28
1	C	278	THR	O-C-N	-5.34	115.20	122.36
1	D	391	PHE	CA-C-O	-5.34	116.79	120.47
1	C	306	THR	O-C-N	-5.34	116.25	122.81
1	C	425	SER	N-CA-CB	-5.34	102.61	111.57
1	A	213	GLU	CA-CB-CG	-5.33	103.43	114.10
1	A	257	ILE	N-CA-CB	5.33	121.03	110.95
1	B	1	MET	CA-C-O	5.33	129.87	120.80
1	C	314	GLU	CB-CG-CD	-5.33	103.53	112.60
1	C	73	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	C	292	ARG	CA-CB-CG	5.33	124.76	114.10
1	C	373	LEU	N-CA-CB	-5.33	101.56	110.99
1	C	463	ASN	CA-C-O	-5.33	113.53	119.34
1	B	400	THR	CA-C-N	-5.33	113.75	122.54
1	B	400	THR	C-N-CA	-5.33	113.75	122.54
1	D	427	ASP	CB-CG-OD1	5.33	130.66	118.40
1	C	222	GLU	N-CA-CB	-5.33	102.70	111.01
1	D	50	LEU	N-CA-C	-5.33	105.56	111.36
1	A	194	ILE	CA-C-O	-5.32	114.26	121.02
1	A	226	GLY	O-C-N	5.32	127.29	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	VAL	N-CA-C	-5.32	104.31	111.44
1	B	360	ARG	CG-CD-NE	-5.32	100.30	112.00
1	B	404	LYS	N-CA-C	-5.32	105.56	111.36
1	C	65	LEU	CA-C-N	-5.32	115.12	122.30
1	C	65	LEU	C-N-CA	-5.32	115.12	122.30
1	C	180	PHE	N-CA-C	-5.32	104.73	111.11
1	D	190	ALA	N-CA-CB	5.32	119.09	110.42
1	A	57	THR	CB-CA-C	-5.31	100.45	109.38
1	C	252	PRO	CB-CA-C	-5.31	104.80	111.71
1	C	301	ALA	N-CA-C	-5.31	105.66	111.82
1	D	89	GLN	CA-C-O	-5.31	116.03	121.87
1	D	402	ASN	CA-CB-CG	-5.31	107.29	112.60
1	B	459	SER	O-C-N	5.30	129.61	122.82
1	D	76	LYS	N-CA-C	5.30	117.71	110.55
1	C	426	THR	CA-C-O	-5.30	115.25	120.82
1	B	201	ILE	O-C-N	5.30	127.22	121.87
1	A	47	ILE	CA-CB-CG1	-5.30	101.39	110.40
1	B	404	LYS	CB-CG-CD	5.30	123.49	111.30
1	C	357	ALA	N-CA-CB	5.30	118.00	110.16
1	D	463	ASN	O-C-N	5.30	128.88	122.20
1	A	85	LEU	O-C-N	5.29	128.87	122.94
1	A	393	ASP	CA-C-O	-5.29	114.36	120.24
1	B	229	ASN	CA-CB-CG	-5.29	107.31	112.60
1	B	315	SER	CA-CB-OG	5.29	121.69	111.10
1	D	77	LEU	CA-C-O	5.29	127.09	121.11
1	A	173	LYS	N-CA-C	-5.29	105.62	111.71
1	A	196	LYS	CA-C-N	-5.29	112.66	120.28
1	A	196	LYS	C-N-CA	-5.29	112.66	120.28
1	D	180	PHE	N-CA-C	-5.28	105.52	111.28
1	D	374	ILE	CA-C-O	5.28	125.94	120.39
1	B	73	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	143	ILE	CA-CB-CG1	-5.28	101.42	110.40
1	B	155	ASN	N-CA-CB	-5.28	101.57	110.49
1	B	442	LEU	CA-C-O	5.28	125.46	119.18
1	C	240	ILE	N-CA-C	5.28	117.36	108.81
1	A	244	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	B	297	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	53	VAL	CA-C-N	-5.27	113.69	120.65
1	C	53	VAL	C-N-CA	-5.27	113.69	120.65
1	C	201	ILE	CB-CG1-CD1	5.27	124.87	113.80
1	A	314	GLU	N-CA-CB	5.27	118.34	110.22
1	B	342	ARG	CA-C-O	-5.27	113.93	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	THR	CA-C-O	5.27	125.59	119.32
1	B	261	LYS	CA-C-O	5.26	126.86	121.07
1	C	210	HIS	CB-CG-CD2	5.26	138.04	131.20
1	C	89	GLN	CA-C-N	-5.26	114.81	122.65
1	C	89	GLN	C-N-CA	-5.26	114.81	122.65
1	B	324	ALA	CA-C-O	-5.26	114.84	120.42
1	B	340	ASN	CA-C-O	-5.26	115.46	121.40
1	D	100	ILE	CA-CB-CG1	-5.26	101.46	110.40
1	A	82	ASP	CA-CB-CG	-5.26	107.34	112.60
1	D	468	HIS	CA-C-N	-5.26	116.31	122.93
1	D	468	HIS	C-N-CA	-5.26	116.31	122.93
1	D	195	ARG	CA-C-N	-5.25	112.00	121.62
1	D	195	ARG	C-N-CA	-5.25	112.00	121.62
1	D	435	GLU	CA-C-O	5.25	126.85	121.07
1	D	320	TYR	CB-CG-CD1	-5.25	112.93	120.80
1	B	87	ALA	N-CA-CB	-5.24	101.36	109.69
1	A	99	VAL	CA-C-N	5.24	130.24	123.11
1	A	99	VAL	C-N-CA	5.24	130.24	123.11
1	D	246	ASP	CA-C-N	-5.24	113.26	120.28
1	D	246	ASP	C-N-CA	-5.24	113.26	120.28
1	B	357	ALA	CA-C-N	-5.24	113.96	120.56
1	B	357	ALA	C-N-CA	-5.24	113.96	120.56
1	B	386	ALA	CA-C-O	-5.24	113.94	119.97
1	A	335	THR	N-CA-C	-5.24	105.25	111.69
1	D	172	GLU	OE1-CD-OE2	-5.24	110.33	122.90
1	D	225	GLU	OE1-CD-OE2	5.23	135.46	122.90
1	C	149	ASN	CB-CG-OD1	5.23	131.26	120.80
1	D	96	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	71	GLU	O-C-N	-5.23	117.09	123.10
1	A	121	ASN	CA-C-O	-5.23	116.01	121.55
1	A	334	ARG	CA-C-N	-5.23	111.64	120.58
1	A	334	ARG	C-N-CA	-5.23	111.64	120.58
1	B	132	MET	CB-CG-SD	-5.23	97.02	112.70
1	B	186	VAL	CA-CB-CG1	-5.23	101.51	110.40
1	D	135	THR	O-C-N	5.23	129.78	122.36
1	B	240	ILE	N-CA-CB	-5.23	102.69	112.36
1	B	296	GLY	CA-C-O	5.23	126.20	120.66
1	D	166	ALA	CA-C-O	-5.23	113.16	119.59
1	D	463	ASN	N-CA-CB	-5.22	102.60	111.27
1	A	110	TYR	CB-CA-C	-5.22	102.53	111.41
1	D	258	PHE	CA-C-N	-5.22	113.65	120.44
1	D	258	PHE	C-N-CA	-5.22	113.65	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	ILE	CB-CA-C	-5.22	104.01	111.31
1	B	157	GLY	CA-C-O	-5.21	116.89	121.58
1	C	87	ALA	CB-CA-C	-5.21	100.41	109.64
1	D	155	ASN	CB-CG-OD1	-5.21	110.38	120.80
1	B	60	THR	CA-C-O	-5.21	115.22	121.11
1	B	300	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	206	HIS	N-CA-C	-5.21	105.29	111.69
1	B	332	CYS	CA-C-O	5.20	126.47	120.90
1	D	123	VAL	CG1-CB-CG2	5.20	122.25	110.80
1	A	244	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	385	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	B	304	ASP	N-CA-C	-5.20	106.03	112.38
1	B	216	HIS	CA-C-O	-5.20	114.76	120.69
1	C	307	ASP	CA-C-N	-5.20	113.79	122.21
1	C	307	ASP	C-N-CA	-5.20	113.79	122.21
1	A	323	GLU	N-CA-CB	5.20	117.85	110.16
1	A	382	LYS	N-CA-C	5.20	116.94	111.28
1	A	389	LYS	CB-CA-C	-5.20	101.02	110.63
1	D	324	ALA	CA-C-O	-5.19	115.35	120.70
1	D	40	TYR	CA-C-N	-5.19	112.92	120.29
1	D	40	TYR	C-N-CA	-5.19	112.92	120.29
1	A	197	ARG	CA-CB-CG	5.19	124.48	114.10
1	D	78	GLU	O-C-N	5.19	130.18	123.07
1	A	87	ALA	N-CA-CB	-5.19	101.44	109.69
1	A	317	LYS	N-CA-CB	-5.19	102.81	111.06
1	D	405	THR	CB-CA-C	5.18	119.02	110.88
1	A	127	ASP	O-C-N	5.18	129.08	122.86
1	D	32	ARG	CA-C-N	-5.18	115.79	123.05
1	D	32	ARG	C-N-CA	-5.18	115.79	123.05
1	D	234	LEU	O-C-N	5.18	127.61	122.12
1	A	42	GLU	O-C-N	5.18	127.69	122.09
1	C	24	LEU	N-CA-C	-5.18	105.06	111.33
1	C	202	GLU	O-C-N	-5.18	115.90	122.27
1	D	181	GLY	O-C-N	5.18	127.15	122.18
1	A	295	ALA	N-CA-CB	5.17	117.73	110.12
1	C	167	LEU	CA-CB-CG	-5.17	98.19	116.30
1	B	29	ASN	CB-CA-C	-5.17	101.06	109.13
1	B	228	ASN	CA-C-O	5.17	125.94	120.10
1	C	179	ILE	CA-CB-CG1	-5.17	101.61	110.40
1	D	356	GLU	CB-CA-C	-5.17	102.54	110.81
1	A	385	ARG	CA-CB-CG	-5.17	103.76	114.10
1	B	365	THR	CA-CB-OG1	-5.17	101.85	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	GLU	N-CA-CB	-5.17	103.40	111.56
1	A	199	ASP	O-C-N	-5.17	116.75	122.07
1	D	78	GLU	CG-CD-OE2	-5.17	106.52	118.40
1	B	102	ASN	CB-CG-ND2	5.16	124.15	116.40
1	C	215	ILE	O-C-N	5.16	128.84	122.95
1	A	217	ILE	N-CA-CB	5.16	117.97	111.46
1	C	144	CYS	CB-CA-C	5.16	124.03	111.65
1	B	306	THR	OG1-CB-CG2	5.16	119.62	109.30
1	D	112	GLY	CA-C-N	-5.16	113.37	120.28
1	D	112	GLY	C-N-CA	-5.16	113.37	120.28
1	B	204	ARG	O-C-N	5.16	128.61	122.27
1	C	99	VAL	CA-C-N	5.16	130.12	123.11
1	C	99	VAL	C-N-CA	5.16	130.12	123.11
1	A	328	MET	CB-CA-C	-5.16	101.09	110.63
1	D	133	GLU	CA-C-N	-5.16	114.58	121.80
1	D	133	GLU	C-N-CA	-5.16	114.58	121.80
1	C	467	VAL	CA-C-O	-5.15	114.47	121.02
1	B	411	LEU	CA-C-O	-5.15	112.35	119.05
1	A	382	LYS	CA-CB-CG	-5.15	103.80	114.10
1	D	293	ALA	CA-C-O	5.15	126.23	120.82
1	C	225	GLU	CA-C-O	5.15	126.23	120.82
1	D	254	GLU	O-C-N	5.15	129.56	122.46
1	D	314	GLU	CA-C-N	-5.15	114.26	122.29
1	D	314	GLU	C-N-CA	-5.15	114.26	122.29
1	A	402	ASN	O-C-N	-5.14	117.22	123.13
1	B	402	ASN	CA-CB-CG	-5.14	107.46	112.60
1	C	125	VAL	O-C-N	5.14	128.60	123.10
1	B	141	LYS	N-CA-C	5.14	117.82	109.24
1	D	244	ARG	CA-C-O	-5.13	115.01	121.02
1	C	463	ASN	CB-CG-OD1	5.13	131.06	120.80
1	B	164	SER	CA-CB-OG	5.12	121.35	111.10
1	C	54	MET	CG-SD-CE	-5.12	89.63	100.90
1	A	418	GLN	CG-CD-NE2	-5.12	108.72	116.40
1	A	462	THR	CA-C-N	-5.12	113.59	122.14
1	A	462	THR	C-N-CA	-5.12	113.59	122.14
1	C	145	LYS	CD-CE-NZ	-5.12	95.53	111.90
1	A	223	ASN	CA-CB-CG	-5.12	107.48	112.60
1	D	60	THR	O-C-N	5.12	129.84	123.19
1	D	268	ILE	CB-CA-C	-5.11	105.24	112.14
1	D	415	VAL	CB-CA-C	-5.11	103.89	110.84
1	B	151	ASP	O-C-N	5.11	129.32	123.29
1	B	439	GLN	N-CA-CB	5.11	118.08	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ILE	CA-C-O	-5.10	115.12	120.27
1	A	452	VAL	CB-CA-C	-5.10	102.97	110.82
1	B	163	VAL	N-CA-CB	5.10	117.60	110.56
1	C	164	SER	CA-CB-OG	5.10	121.30	111.10
1	D	385	ARG	CA-C-N	5.10	128.06	120.31
1	D	385	ARG	C-N-CA	5.10	128.06	120.31
1	A	422	GLU	CB-CG-CD	5.10	121.27	112.60
1	B	44	GLY	CA-C-N	-5.10	113.05	120.29
1	B	44	GLY	C-N-CA	-5.10	113.05	120.29
1	C	292	ARG	CD-NE-CZ	5.10	131.53	124.40
1	A	170	LEU	CA-C-O	-5.09	115.01	120.46
1	C	435	GLU	OE1-CD-OE2	5.09	135.13	122.90
1	A	74	THR	N-CA-C	-5.09	102.98	110.52
1	B	188	PHE	CA-C-O	-5.09	115.15	121.06
1	A	18	GLU	O-C-N	5.09	127.52	122.12
1	A	165	ILE	N-CA-C	5.09	116.29	108.71
1	C	398	ALA	CA-C-N	-5.09	113.99	122.64
1	C	398	ALA	C-N-CA	-5.09	113.99	122.64
1	A	199	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	180	PHE	CA-C-O	-5.08	115.46	120.90
1	B	425	SER	N-CA-C	5.08	115.87	108.14
1	A	232	GLU	CG-CD-OE2	-5.08	106.71	118.40
1	A	314	GLU	CA-C-N	-5.08	114.25	122.23
1	A	314	GLU	C-N-CA	-5.08	114.25	122.23
1	C	360	ARG	CA-C-O	5.08	125.94	120.55
1	A	160	LEU	O-C-N	5.08	126.34	121.31
1	C	225	GLU	O-C-N	5.08	127.30	122.07
1	D	452	VAL	CB-CA-C	-5.08	103.00	110.82
1	A	187	ASP	CA-C-O	5.08	125.21	119.27
1	B	409	LEU	O-C-N	-5.08	115.79	122.39
1	D	178	LEU	CD1-CG-CD2	-5.08	99.63	110.80
1	D	437	ALA	N-CA-C	-5.08	105.64	111.07
1	A	420	VAL	CA-CB-CG1	5.08	119.03	110.40
1	B	463	ASN	N-CA-CB	-5.08	102.84	111.27
1	A	405	THR	CA-C-O	-5.08	115.47	120.70
1	B	57	THR	O-C-N	5.07	128.15	122.27
1	C	311	LEU	CB-CA-C	-5.07	101.39	109.75
1	D	307	ASP	OD1-CG-OD2	5.07	135.07	122.90
1	A	325	VAL	CA-C-N	5.07	127.07	120.28
1	A	325	VAL	C-N-CA	5.07	127.07	120.28
1	A	266	LYS	CA-C-O	-5.07	114.38	120.10
1	C	356	GLU	CA-CB-CG	5.07	124.23	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	LYS	CA-C-O	5.07	125.83	120.36
1	B	216	HIS	CA-CB-CG	-5.06	108.74	113.80
1	D	425	SER	N-CA-C	5.06	115.83	108.14
1	A	2	LYS	CA-C-O	5.06	127.75	122.03
1	B	389	LYS	CB-CA-C	-5.06	100.36	110.42
1	B	212	GLY	CA-C-N	5.06	130.39	120.99
1	B	212	GLY	C-N-CA	5.06	130.39	120.99
1	D	228	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	76	LYS	O-C-N	5.05	128.61	122.85
1	A	260	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	C	452	VAL	O-C-N	5.05	128.63	123.18
1	C	11	GLY	CA-C-O	5.05	128.74	121.52
1	A	45	GLN	CG-CD-NE2	5.04	123.97	116.40
1	B	146	VAL	CA-C-N	-5.04	112.68	122.06
1	B	146	VAL	C-N-CA	-5.04	112.68	122.06
1	C	169	ALA	O-C-N	5.04	129.11	122.30
1	D	28	MET	CB-CA-C	-5.04	102.03	109.90
1	A	144	CYS	CA-C-O	-5.04	115.64	121.49
1	A	196	LYS	CB-CG-CD	5.04	122.89	111.30
1	D	339	MET	N-CA-CB	-5.04	103.23	110.44
1	A	83	VAL	O-C-N	5.04	128.49	123.10
1	D	194	ILE	O-C-N	-5.04	117.22	122.81
1	B	33	LEU	CA-C-O	-5.03	115.08	120.46
1	B	267	CYS	N-CA-C	5.03	116.45	111.07
1	C	402	ASN	O-C-N	-5.03	117.48	123.22
1	A	300	ASN	O-C-N	-5.03	116.08	122.27
1	A	433	GLY	CA-C-N	-5.03	113.60	120.44
1	A	433	GLY	C-N-CA	-5.03	113.60	120.44
1	A	435	GLU	OE1-CD-OE2	5.03	134.97	122.90
1	D	127	ASP	CA-CB-CG	-5.03	107.57	112.60
1	D	230	PHE	CA-C-O	5.03	127.70	120.51
1	A	67	THR	N-CA-CB	5.03	117.55	110.36
1	A	78	GLU	N-CA-CB	5.03	117.53	109.28
1	A	303	LEU	N-CA-CB	5.03	118.07	110.28
1	B	255	GLU	CA-CB-CG	-5.03	104.04	114.10
1	B	383	SER	CB-CA-C	5.03	120.64	110.38
1	D	385	ARG	N-CA-C	5.03	117.65	111.82
1	B	96	ASP	CB-CA-C	-5.03	103.12	111.41
1	B	408	GLN	N-CA-CB	5.03	117.96	110.22
1	D	119	VAL	O-C-N	5.03	127.66	122.79
1	B	295	ALA	O-C-N	5.02	127.45	122.12
1	B	127	ASP	N-CA-CB	5.02	118.80	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	SER	CA-C-N	5.02	131.25	121.41
1	B	453	SER	C-N-CA	5.02	131.25	121.41
1	C	295	ALA	N-CA-CB	5.02	117.50	110.12
1	B	186	VAL	CA-C-O	-5.02	117.05	121.97
1	D	118	SER	N-CA-CB	-5.02	102.19	111.52
1	D	390	TYR	CA-C-N	-5.02	118.28	123.10
1	D	390	TYR	C-N-CA	-5.02	118.28	123.10
1	C	133	GLU	CB-CA-C	-5.01	101.06	109.48
1	D	388	ARG	N-CA-CB	-5.01	101.79	110.32
1	B	276	THR	CA-C-O	5.01	125.75	120.54
1	A	463	ASN	N-CA-CB	-5.01	103.17	111.49
1	D	50	LEU	CA-C-N	-5.01	113.57	120.28
1	D	50	LEU	C-N-CA	-5.01	113.57	120.28
1	D	389	LYS	CB-CG-CD	-5.01	99.78	111.30
1	B	216	HIS	CA-C-N	-5.01	116.62	122.93
1	B	216	HIS	C-N-CA	-5.01	116.62	122.93
1	B	222	GLU	CA-C-O	5.01	124.69	119.03
1	B	60	THR	CB-CA-C	-5.01	99.47	109.33
1	D	439	GLN	OE1-CD-NE2	5.01	127.61	122.60
1	D	325	VAL	CA-CB-CG2	-5.00	101.89	110.40
1	B	224	GLN	O-C-N	5.00	127.42	122.12
1	C	398	ALA	N-CA-CB	5.00	118.41	110.55
1	C	428	ASP	CA-C-N	5.00	126.98	120.28
1	C	428	ASP	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ASP	Mainchain
1	A	277	ALA	Mainchain
1	B	2	LYS	Mainchain
1	B	223	ASN	Mainchain
1	B	277	ALA	Mainchain
1	B	28	MET	Mainchain
1	C	104	GLU	Sidechain
1	C	138	GLU	Sidechain
1	C	277	ALA	Mainchain
1	D	277	ALA	Mainchain
1	D	3	LYS	Mainchain
1	D	30	VAL	Mainchain
1	D	410	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	D	452	VAL	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	3445	0	3533	189	0
1	B	3445	0	3533	149	0
1	C	3445	0	3533	313	1
1	D	3445	0	3533	151	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	38	0	0	4	0
3	B	55	0	0	2	0
3	C	48	0	0	10	0
3	D	59	0	0	5	0
All	All	14000	0	14132	785	1

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 28.

All (785) 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:C:92:THR:HG22	1:C:105:MET:SD	1.35	1.62
1:C:136:ALA:CB	1:C:143:ILE:CG2	1.82	1.58
1:C:77:LEU:CD1	1:C:154:GLU:HB3	1.33	1.58
1:C:136:ALA:CB	1:C:143:ILE:HG21	1.36	1.51
1:C:92:THR:CG2	1:C:105:MET:SD	2.05	1.45
1:C:136:ALA:HB3	1:C:143:ILE:CG2	0.94	1.41
1:A:88:GLY:HA2	1:A:145:LYS:CE	1.49	1.40
1:A:88:GLY:CA	1:A:145:LYS:HE3	1.52	1.39
1:C:92:THR:O	1:C:105:MET:HB2	1.31	1.26
1:C:106:VAL:CG2	1:C:107:ALA:H	1.36	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:VAL:HA	1:C:134:VAL:CG1	1.67	1.24
1:C:137:ILE:CG1	1:C:142:VAL:HG13	1.68	1.21
1:C:197:ARG:HB3	1:C:232:GLU:HG3	1.19	1.19
1:C:106:VAL:HG22	1:C:107:ALA:N	1.38	1.17
1:C:92:THR:OG1	1:C:143:ILE:HA	1.46	1.16
1:D:354:ILE:N	3:D:2048:HOH:O	1.76	1.14
1:C:137:ILE:HG13	1:C:142:VAL:HG13	1.26	1.12
1:C:77:LEU:HD11	1:C:154:GLU:HB3	1.22	1.12
1:C:77:LEU:CD1	1:C:154:GLU:CB	2.30	1.10
1:C:165:ILE:HG22	1:C:167:LEU:H	1.10	1.10
1:C:77:LEU:HD12	1:C:154:GLU:CB	1.81	1.09
1:A:434:LYS:HG3	1:A:451:MET:HE1	1.32	1.09
1:B:70:PRO:HB2	1:B:167:LEU:HD13	1.25	1.09
1:C:434:LYS:HG3	1:C:451:MET:HE1	1.35	1.08
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.33	1.06
1:A:69:GLY:HA2	1:A:174:ASP:OD2	1.57	1.05
1:C:136:ALA:CB	1:C:143:ILE:HG22	1.62	1.05
1:D:10:ILE:HG12	1:D:31:MET:HG3	1.40	1.03
1:A:118:SER:N	1:A:121:ASN:OD1	1.90	1.03
1:C:113:PHE:CE1	1:C:117:LEU:CD2	2.43	1.02
1:C:119:VAL:HA	1:C:134:VAL:HG12	1.01	1.01
1:C:137:ILE:CG1	1:C:142:VAL:CG1	2.39	1.00
1:C:137:ILE:HG12	1:C:142:VAL:CG1	1.92	1.00
1:C:130:ILE:HG22	1:C:132:MET:HE2	1.41	1.00
1:D:80:GLY:HA2	1:D:154:GLU:OE2	1.60	0.99
1:C:90:THR:HG23	1:C:144:CYS:O	1.61	0.99
1:C:69:GLY:N	1:C:174:ASP:OD2	1.94	0.99
1:C:77:LEU:HD12	1:C:154:GLU:HB3	0.98	0.98
1:A:45:GLN:HB2	3:A:2007:HOH:O	1.63	0.97
1:C:73:ARG:HB2	1:C:109:THR:HG23	1.42	0.97
1:C:191:ALA:O	1:C:220:LYS:HG3	1.63	0.97
1:C:175:LYS:HG2	1:C:206:HIS:CE1	1.98	0.97
1:C:133:GLU:O	1:C:144:CYS:HB3	1.65	0.97
1:A:170:LEU:CD2	1:A:174:ASP:HB3	1.93	0.97
1:C:159:ASN:C	1:C:160:LEU:HD23	1.89	0.97
1:D:50:LEU:HG	1:D:54:MET:HE2	1.46	0.96
1:C:136:ALA:HB3	1:C:143:ILE:HG22	0.99	0.96
1:C:114:THR:HG22	1:C:137:ILE:HG21	1.47	0.96
1:D:140:ASN:OD1	1:D:141:LYS:HG3	1.64	0.96
1:A:51:ARG:HA	1:A:54:MET:HE3	1.43	0.95
1:C:204:ARG:NH2	1:C:238:ASP:OD2	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HG22	1:C:137:ILE:CG2	1.97	0.95
1:D:39:ASP:OD1	1:D:42:GLU:HG3	1.67	0.95
1:D:434:LYS:HG3	1:D:451:MET:HE1	1.47	0.94
1:C:158:VAL:HG12	1:C:160:LEU:HD21	1.47	0.94
1:C:50:LEU:HG	1:C:54:MET:HE2	1.49	0.94
1:C:136:ALA:HB3	1:C:143:ILE:CB	1.97	0.94
1:C:137:ILE:HG12	1:C:142:VAL:HG22	1.46	0.94
1:A:50:LEU:HG	1:A:54:MET:HE2	1.49	0.94
1:C:113:PHE:CE1	1:C:117:LEU:HD21	2.04	0.93
1:C:113:PHE:HE1	1:C:117:LEU:HD21	1.33	0.92
1:C:251:ILE:HB	1:C:252:PRO:HD2	1.51	0.92
1:C:171:ALA:HB3	1:C:174:ASP:HB2	1.47	0.92
1:C:90:THR:CG2	1:C:144:CYS:O	2.17	0.92
1:C:130:ILE:HG22	1:C:132:MET:CE	1.99	0.92
1:C:354:ILE:N	3:C:2036:HOH:O	2.03	0.92
1:C:354:ILE:N	3:C:2035:HOH:O	2.01	0.90
1:B:8:CYS:HB2	1:B:28:MET:HE3	1.52	0.90
1:C:51:ARG:HA	1:C:54:MET:HE3	1.53	0.90
1:B:434:LYS:HG3	1:B:451:MET:HE1	1.51	0.90
1:B:14:THR:HG21	1:B:315:SER:O	1.73	0.89
1:C:133:GLU:O	1:C:144:CYS:CB	2.20	0.89
1:C:137:ILE:HG13	1:C:142:VAL:CG1	2.03	0.88
1:C:92:THR:O	1:C:105:MET:CB	2.21	0.88
1:C:137:ILE:HG12	1:C:142:VAL:CG2	2.03	0.87
1:C:136:ALA:HB2	1:C:143:ILE:HG21	1.52	0.87
1:C:152:LEU:HD12	1:C:153:GLY:O	1.75	0.87
1:C:202:GLU:CG	3:C:2016:HOH:O	2.23	0.87
1:C:137:ILE:HG23	1:C:141:LYS:O	1.74	0.86
1:D:87:ALA:HA	1:D:146:VAL:HG12	1.57	0.86
1:C:137:ILE:HG12	1:C:142:VAL:HG13	1.47	0.86
1:A:191:ALA:O	1:A:220:LYS:HG3	1.75	0.86
1:B:191:ALA:O	1:B:220:LYS:HG3	1.75	0.86
1:C:159:ASN:O	1:C:160:LEU:HD23	1.75	0.86
1:A:10:ILE:CG1	1:A:31:MET:HG3	2.06	0.85
1:B:97:LYS:NZ	1:B:109:THR:O	2.08	0.85
1:C:77:LEU:HD11	1:C:154:GLU:CB	2.01	0.85
1:C:165:ILE:HG22	1:C:167:LEU:N	1.91	0.85
1:D:402:ASN:ND2	1:D:405:THR:H	1.74	0.85
1:C:136:ALA:CA	1:C:143:ILE:HG22	2.07	0.84
1:A:204:ARG:NH2	1:A:238:ASP:OD2	2.08	0.84
1:A:80:GLY:HA2	1:A:154:GLU:OE2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:O	1:C:175:LYS:HE3	1.77	0.83
1:C:73:ARG:HB2	1:C:109:THR:CG2	2.07	0.83
1:B:50:LEU:HG	1:B:54:MET:HE2	1.60	0.83
1:C:10:ILE:HG12	1:C:31:MET:HG3	1.58	0.83
1:D:204:ARG:NH2	1:D:238:ASP:OD2	2.11	0.83
1:C:113:PHE:HE1	1:C:117:LEU:CD2	1.84	0.82
1:C:106:VAL:HG22	1:C:107:ALA:H	0.67	0.82
1:A:99:VAL:HG11	1:A:105:MET:CE	2.10	0.82
1:C:136:ALA:N	1:C:143:ILE:HG22	1.95	0.82
1:B:204:ARG:NH2	1:B:238:ASP:OD2	2.11	0.81
1:C:14:THR:HG21	1:C:315:SER:O	1.79	0.81
1:C:119:VAL:CA	1:C:134:VAL:CG1	2.57	0.81
1:C:434:LYS:CG	1:C:451:MET:HE1	2.10	0.81
1:C:119:VAL:CA	1:C:134:VAL:HG12	1.98	0.81
1:D:8:CYS:HB2	1:D:28:MET:HE3	1.62	0.81
1:C:170:LEU:HD13	1:C:175:LYS:HG3	1.61	0.81
1:C:136:ALA:HB3	1:C:143:ILE:HG21	0.84	0.80
1:A:299:ALA:CB	1:C:257:ILE:HD11	2.12	0.80
1:B:80:GLY:HA2	1:B:154:GLU:OE2	1.80	0.80
1:C:136:ALA:HB2	1:C:143:ILE:CG2	2.09	0.80
1:A:10:ILE:HG12	1:A:31:MET:HG3	1.64	0.79
1:C:155:ASN:O	1:C:156:LYS:HD3	1.82	0.79
1:D:160:LEU:HD12	1:D:165:ILE:CD1	2.13	0.79
1:A:99:VAL:HG11	1:A:105:MET:HE3	1.65	0.79
1:B:10:ILE:HG12	1:B:31:MET:HG3	1.63	0.78
1:D:402:ASN:HD22	1:D:405:THR:H	1.29	0.78
1:A:171:ALA:HB3	1:A:174:ASP:CG	2.09	0.78
1:C:202:GLU:HG2	3:C:2016:HOH:O	1.82	0.77
1:C:173:LYS:N	3:C:2012:HOH:O	2.18	0.77
1:D:140:ASN:OD1	1:D:141:LYS:HE3	1.84	0.77
1:A:135:THR:OG1	1:A:143:ILE:HG22	1.85	0.77
1:B:170:LEU:CD2	1:B:174:ASP:HB3	2.15	0.77
1:B:10:ILE:CG1	1:B:31:MET:HG3	2.13	0.76
1:C:92:THR:HG1	1:C:143:ILE:HA	1.51	0.76
1:D:191:ALA:O	1:D:220:LYS:HG3	1.85	0.75
1:D:334:ARG:HD2	1:D:337:ARG:NH1	2.03	0.74
1:A:117:LEU:HD12	1:A:121:ASN:OD1	1.88	0.74
1:D:10:ILE:CG1	1:D:31:MET:HG3	2.17	0.74
1:A:434:LYS:HG3	1:A:451:MET:CE	2.16	0.74
1:C:142:VAL:HG12	1:C:143:ILE:H	1.52	0.73
1:D:51:ARG:HA	1:D:54:MET:HE3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:HG12	1:C:143:ILE:N	2.02	0.73
1:C:158:VAL:CG1	1:C:160:LEU:HD21	2.17	0.73
1:A:402:ASN:C	1:A:402:ASN:HD22	1.97	0.73
1:C:197:ARG:HB3	1:C:232:GLU:CG	2.10	0.73
1:C:92:THR:HG21	1:C:105:MET:SD	2.25	0.73
1:D:170:LEU:CD2	1:D:174:ASP:HB3	2.19	0.73
1:C:75:MET:HG3	1:C:107:ALA:HB3	1.70	0.72
1:C:113:PHE:CD1	1:C:117:LEU:CD2	2.72	0.72
1:C:188:PHE:CD1	1:C:216:HIS:HB2	2.24	0.72
1:C:244:ARG:NH1	1:C:278:THR:O	2.22	0.72
1:B:402:ASN:HD22	1:B:405:THR:H	1.38	0.72
1:A:171:ALA:O	1:A:174:ASP:HB2	1.90	0.72
1:B:402:ASN:ND2	1:B:405:THR:H	1.89	0.71
1:C:10:ILE:CG1	1:C:31:MET:HG3	2.20	0.71
1:C:86:LYS:O	1:C:89:GLN:HB3	1.91	0.71
1:C:106:VAL:HG22	1:C:107:ALA:CA	2.20	0.71
1:C:119:VAL:HA	1:C:134:VAL:HG11	1.72	0.70
1:D:402:ASN:HA	3:D:2053:HOH:O	1.90	0.70
1:A:188:PHE:CD1	1:A:216:HIS:HB2	2.26	0.70
1:B:23:MET:CE	1:B:325:VAL:HG21	2.21	0.70
1:D:50:LEU:HG	1:D:54:MET:CE	2.20	0.70
1:D:358:VAL:HG21	1:D:463:ASN:HA	1.72	0.70
1:C:75:MET:CG	1:C:107:ALA:HB3	2.21	0.70
1:A:89:GLN:HG3	1:A:90:THR:O	1.90	0.70
1:D:170:LEU:HD22	1:D:174:ASP:HB3	1.73	0.70
1:C:106:VAL:HG22	1:C:107:ALA:CB	2.22	0.70
1:C:169:ALA:HB3	3:C:2017:HOH:O	1.91	0.69
1:C:92:THR:C	1:C:105:MET:HB2	2.17	0.69
1:D:160:LEU:HD12	1:D:165:ILE:HD13	1.74	0.69
1:A:10:ILE:HG13	1:A:31:MET:HG3	1.72	0.69
1:C:175:LYS:HG2	1:C:206:HIS:HE1	1.55	0.69
1:D:251:ILE:HB	1:D:252:PRO:HD2	1.75	0.69
1:A:244:ARG:NH1	1:A:278:THR:O	2.26	0.68
1:B:358:VAL:HG21	1:B:463:ASN:HA	1.75	0.68
1:A:93:PHE:CE2	1:A:123:VAL:HG11	2.29	0.68
1:A:75:MET:HG3	1:A:107:ALA:HB3	1.75	0.68
1:D:376:VAL:HG22	1:D:452:VAL:HB	1.75	0.68
1:A:96:ASP:O	1:A:98:SER:N	2.26	0.68
1:B:86:LYS:O	1:B:89:GLN:HB3	1.94	0.68
1:A:358:VAL:HG21	1:A:463:ASN:HA	1.76	0.68
1:D:80:GLY:CA	1:D:154:GLU:OE2	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASP:OD1	1:B:42:GLU:HG3	1.92	0.68
1:C:138:GLU:OE1	1:C:138:GLU:HG2	1.94	0.68
1:B:434:LYS:CG	1:B:451:MET:HE1	2.22	0.67
1:C:138:GLU:O	1:C:141:LYS:HB2	1.93	0.67
1:A:44:GLY:O	3:A:2006:HOH:O	2.12	0.67
1:C:92:THR:OG1	1:C:143:ILE:HG13	1.93	0.67
1:C:108:VAL:HG21	1:C:113:PHE:CD2	2.29	0.67
1:C:135:THR:OG1	1:C:143:ILE:HG23	1.95	0.67
1:D:74:THR:O	1:D:155:ASN:HA	1.94	0.67
1:C:130:ILE:CG2	1:C:132:MET:CE	2.72	0.67
1:B:131:GLY:C	1:B:132:MET:HG3	2.19	0.67
1:A:175:LYS:HG2	1:A:206:HIS:CE1	2.30	0.66
1:C:251:ILE:HB	1:C:252:PRO:CD	2.24	0.66
1:A:135:THR:OG1	1:A:143:ILE:O	2.13	0.66
1:B:23:MET:HE2	1:B:325:VAL:HG21	1.77	0.66
1:D:69:GLY:HA2	1:D:174:ASP:OD2	1.96	0.66
1:B:125:VAL:HG12	1:B:126:ASP:N	2.11	0.66
1:B:92:THR:O	1:B:105:MET:HB2	1.96	0.66
1:B:334:ARG:HD2	1:B:337:ARG:NH1	2.11	0.66
1:D:31:MET:HE2	1:D:50:LEU:HD22	1.78	0.66
1:C:170:LEU:HD13	1:C:175:LYS:CG	2.26	0.65
1:A:124:LEU:HD23	1:A:131:GLY:HA2	1.78	0.65
1:A:124:LEU:HD23	1:A:131:GLY:CA	2.27	0.65
1:B:131:GLY:C	1:B:132:MET:CG	2.70	0.65
1:D:2:LYS:HE2	1:D:6:ILE:HD12	1.77	0.65
1:C:39:ASP:OD1	1:C:42:GLU:HG3	1.97	0.65
1:A:197:ARG:HB3	1:A:232:GLU:HG3	1.78	0.64
1:A:383:SER:HB3	1:A:462:THR:OG1	1.97	0.64
1:C:113:PHE:CE1	1:C:117:LEU:HD23	2.32	0.64
1:C:138:GLU:OE1	1:C:138:GLU:CG	2.45	0.64
1:B:125:VAL:HG22	1:B:158:VAL:HG22	1.78	0.64
1:C:159:ASN:C	1:C:161:PRO:HD3	2.22	0.64
1:B:125:VAL:CG1	1:B:126:ASP:N	2.60	0.64
1:C:191:ALA:HB1	1:C:203:ILE:CD1	2.27	0.64
1:D:191:ALA:HB1	1:D:203:ILE:CD1	2.27	0.64
1:C:104:GLU:O	1:C:105:MET:HB3	1.97	0.64
1:C:158:VAL:HG12	1:C:160:LEU:CD2	2.25	0.64
1:C:376:VAL:HG22	1:C:452:VAL:HB	1.80	0.63
1:C:92:THR:HG23	1:C:105:MET:SD	2.31	0.63
1:C:175:LYS:CD	1:C:206:HIS:HE1	2.11	0.63
1:C:133:GLU:N	1:C:147:LEU:HD21	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ALA:CB	1:B:203:ILE:CD1	2.77	0.63
1:A:197:ARG:CB	1:A:232:GLU:HG3	2.29	0.63
1:D:402:ASN:HD22	1:D:402:ASN:C	2.05	0.63
1:C:137:ILE:CG2	1:C:142:VAL:HG22	2.28	0.63
1:C:137:ILE:N	3:C:2010:HOH:O	2.31	0.63
1:A:163:VAL:O	1:A:165:ILE:HD12	1.99	0.62
1:A:434:LYS:CG	1:A:451:MET:HE1	2.20	0.62
1:B:50:LEU:HG	1:B:54:MET:CE	2.29	0.62
1:B:402:ASN:HB3	1:B:405:THR:HB	1.81	0.62
1:B:118:SER:O	1:B:121:ASN:HB2	1.99	0.62
1:B:318:GLY:HA3	3:B:2040:HOH:O	2.00	0.62
1:C:136:ALA:H	1:C:143:ILE:HG22	1.62	0.62
1:D:239:GLY:C	1:D:240:ILE:HG12	2.23	0.62
1:C:358:VAL:HG21	1:C:463:ASN:HA	1.82	0.62
1:B:197:ARG:HB3	1:B:232:GLU:HG3	1.81	0.62
1:B:251:ILE:HB	1:B:252:PRO:HD2	1.82	0.62
1:B:284:MET:HA	1:B:287:ASN:O	2.00	0.62
1:D:191:ALA:CB	1:D:203:ILE:CD1	2.77	0.62
1:B:267:CYS:HB3	1:B:272:LYS:O	2.00	0.61
1:C:106:VAL:CG2	1:C:107:ALA:N	2.13	0.61
1:B:376:VAL:HG22	1:B:452:VAL:HB	1.81	0.61
1:C:75:MET:CG	1:C:107:ALA:CB	2.77	0.61
1:D:31:MET:HE2	1:D:50:LEU:CD2	2.30	0.61
1:C:428:ASP:OD1	1:C:431:ARG:NH1	2.33	0.61
1:B:299:ALA:HB1	1:D:257:ILE:HD11	1.81	0.61
1:D:378:THR:OG1	2:D:704:SO4:O3	2.14	0.61
1:B:257:ILE:HD11	1:D:299:ALA:HB1	1.83	0.61
1:C:85:LEU:N	1:C:85:LEU:HD23	2.16	0.61
1:C:92:THR:HG21	1:C:143:ILE:HD11	1.82	0.61
1:A:193:PHE:CE2	1:A:195:ARG:HD3	2.36	0.61
1:A:96:ASP:C	1:A:98:SER:H	2.09	0.60
1:C:77:LEU:HD11	1:C:154:GLU:CA	2.31	0.60
1:D:86:LYS:O	1:D:89:GLN:HB3	2.00	0.60
1:C:175:LYS:CG	1:C:206:HIS:CE1	2.81	0.60
1:B:75:MET:HG3	1:B:107:ALA:O	2.01	0.60
1:B:155:ASN:C	1:B:156:LYS:HG2	2.27	0.60
1:D:160:LEU:HB2	1:D:163:VAL:HB	1.82	0.60
1:C:111:GLU:OE2	1:C:111:GLU:HG2	2.01	0.60
1:C:155:ASN:C	1:C:156:LYS:HD3	2.26	0.60
1:D:164:SER:C	1:D:165:ILE:HG13	2.25	0.60
1:C:136:ALA:HB3	1:C:143:ILE:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:THR:HG21	1:D:302:ILE:HG12	1.84	0.60
1:A:69:GLY:CA	1:A:174:ASP:OD2	2.44	0.60
1:A:170:LEU:HD22	1:A:174:ASP:CB	2.22	0.59
1:C:140:ASN:OD1	1:C:141:LYS:HE3	2.02	0.59
1:B:85:LEU:HD11	1:B:91:PHE:CE1	2.38	0.59
1:B:244:ARG:NH1	1:B:278:THR:O	2.36	0.59
1:D:201:ILE:O	1:D:205:GLU:HG3	2.02	0.59
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.84	0.59
1:C:74:THR:HG22	1:C:93:PHE:HE1	1.66	0.59
1:A:23:MET:CE	1:A:325:VAL:HG21	2.32	0.59
1:A:99:VAL:HG11	1:A:105:MET:HE2	1.84	0.59
1:B:170:LEU:HD23	1:B:174:ASP:HB3	1.83	0.59
1:C:111:GLU:OE2	1:C:111:GLU:CG	2.51	0.59
1:D:23:MET:CE	1:D:325:VAL:HG21	2.33	0.59
1:A:74:THR:O	1:A:155:ASN:HA	2.02	0.59
1:A:255:GLU:CD	1:C:334:ARG:HH11	2.10	0.59
1:C:90:THR:HG22	1:C:144:CYS:O	2.00	0.59
1:C:106:VAL:HG22	1:C:107:ALA:HB3	1.84	0.58
1:A:321:PRO:HG2	1:A:322:LEU:H	1.68	0.58
1:D:373:LEU:HD11	1:D:397:LEU:HB2	1.85	0.58
1:B:191:ALA:CB	1:B:203:ILE:HD12	2.33	0.58
1:B:387:VAL:HG12	1:B:396:ILE:CD1	2.34	0.58
1:C:311:LEU:HD22	1:C:314:GLU:HB2	1.84	0.58
1:A:31:MET:HE2	1:A:50:LEU:HD22	1.85	0.58
1:B:92:THR:HG23	1:B:142:VAL:O	2.03	0.58
1:C:152:LEU:CD1	1:C:153:GLY:O	2.51	0.58
1:D:375:VAL:HG22	1:D:397:LEU:HB3	1.85	0.58
1:A:14:THR:HG21	1:A:315:SER:O	2.03	0.58
1:A:88:GLY:O	1:A:145:LYS:HD2	2.03	0.58
1:B:14:THR:CG2	1:B:315:SER:O	2.51	0.58
1:C:119:VAL:HG22	1:C:135:THR:C	2.29	0.58
1:C:197:ARG:CB	1:C:232:GLU:HG3	2.13	0.58
1:A:23:MET:HE2	1:A:325:VAL:HG21	1.85	0.58
1:A:299:ALA:HB1	1:C:257:ILE:HD11	1.86	0.58
1:B:74:THR:O	1:B:155:ASN:HA	2.04	0.58
1:C:65:LEU:C	1:C:65:LEU:HD23	2.28	0.58
1:C:170:LEU:HD22	1:C:174:ASP:HB3	1.84	0.58
1:D:110:TYR:OH	1:D:116:ASP:OD2	2.17	0.57
1:B:170:LEU:HD22	1:B:174:ASP:HB3	1.84	0.57
1:D:230:PHE:CE1	1:D:263:MET:HG2	2.39	0.57
1:A:191:ALA:HB1	1:A:203:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HH11	1:C:255:GLU:CD	2.12	0.57
1:C:175:LYS:CG	1:C:206:HIS:HE1	2.16	0.57
1:B:114:THR:HG22	1:B:142:VAL:HG23	1.87	0.57
1:C:202:GLU:OE1	3:C:2015:HOH:O	2.18	0.57
1:C:373:LEU:HD12	1:C:395:THR:O	2.03	0.57
1:A:140:ASN:C	1:A:141:LYS:HG2	2.30	0.57
1:B:402:ASN:HD22	1:B:402:ASN:C	2.13	0.57
1:A:376:VAL:HG22	1:A:452:VAL:HB	1.86	0.57
1:C:284:MET:HA	1:C:287:ASN:O	2.04	0.57
1:A:113:PHE:HD2	1:A:142:VAL:HG21	1.68	0.56
1:B:65:LEU:C	1:B:65:LEU:HD23	2.30	0.56
1:C:430:TYR:O	1:C:434:LYS:HG3	2.05	0.56
1:A:110:TYR:OH	1:A:166:ALA:HB3	2.05	0.56
1:A:251:ILE:HB	1:A:252:PRO:HD2	1.88	0.56
1:B:132:MET:HA	1:B:147:LEU:HG	1.87	0.56
1:B:133:GLU:O	1:B:144:CYS:HA	2.05	0.56
1:B:140:ASN:OD1	1:B:141:LYS:HG3	2.05	0.56
1:B:191:ALA:HB1	1:B:203:ILE:CD1	2.36	0.56
1:D:229:ASN:O	1:D:230:PHE:C	2.48	0.56
1:D:160:LEU:HD12	1:D:165:ILE:HD11	1.88	0.56
1:D:274:VAL:HG13	1:D:274:VAL:O	2.06	0.56
1:A:206:HIS:O	1:A:207:LEU:C	2.48	0.56
1:C:133:GLU:O	1:C:144:CYS:CA	2.54	0.56
1:D:160:LEU:N	3:D:2020:HOH:O	2.13	0.56
1:B:387:VAL:HG12	1:B:396:ILE:HD11	1.86	0.56
1:C:75:MET:HG3	1:C:107:ALA:CB	2.34	0.56
1:A:257:ILE:HD11	1:C:299:ALA:CB	2.36	0.55
1:C:31:MET:HE2	1:C:63:ILE:HG12	1.87	0.55
1:C:142:VAL:CG1	1:C:143:ILE:H	2.17	0.55
1:C:191:ALA:CB	1:C:203:ILE:HD13	2.36	0.55
1:A:39:ASP:OD1	1:A:42:GLU:HG3	2.05	0.55
1:C:83:VAL:HG21	1:C:103:SER:HA	1.88	0.55
1:D:159:ASN:CG	1:D:249:VAL:HG11	2.31	0.55
1:A:73:ARG:O	1:A:109:THR:HG23	2.05	0.55
1:A:402:ASN:ND2	1:A:405:THR:H	2.04	0.55
1:C:198:SER:O	1:C:202:GLU:HG3	2.06	0.55
1:D:17:GLU:OE1	1:D:56:LYS:NZ	2.40	0.55
1:B:73:ARG:HA	1:B:156:LYS:O	2.07	0.55
1:C:83:VAL:HG23	1:C:85:LEU:CD2	2.36	0.55
1:C:133:GLU:C	1:C:144:CYS:HB3	2.31	0.55
1:D:159:ASN:HA	3:D:2020:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:CD2	1:A:142:VAL:HG21	2.42	0.54
1:A:354:ILE:N	3:A:2032:HOH:O	2.40	0.54
1:A:257:ILE:HD11	1:C:299:ALA:HB1	1.89	0.54
1:C:133:GLU:O	1:C:144:CYS:HA	2.07	0.54
1:A:171:ALA:HB3	1:A:174:ASP:OD2	2.07	0.54
1:B:281:LEU:O	1:B:314:GLU:HG2	2.07	0.54
1:D:391:PHE:N	1:D:392:PRO:CD	2.70	0.54
1:B:19:MET:O	1:B:20:LEU:C	2.49	0.54
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.06	0.54
1:C:383:SER:HB3	1:C:462:THR:OG1	2.07	0.54
1:C:77:LEU:HD12	1:C:154:GLU:CG	2.36	0.54
1:D:262:MET:O	1:D:266:LYS:HG3	2.08	0.54
1:A:19:MET:O	1:A:22:LYS:N	2.41	0.53
1:C:167:LEU:HD22	1:C:168:PRO:HD2	1.89	0.53
1:C:191:ALA:CB	1:C:203:ILE:CD1	2.86	0.53
1:C:75:MET:HG2	1:C:107:ALA:O	2.07	0.53
1:A:94:THR:HG21	1:A:105:MET:HE3	1.88	0.53
1:A:133:GLU:HB2	1:A:147:LEU:HD21	1.91	0.53
1:A:284:MET:HA	1:A:287:ASN:O	2.09	0.53
1:B:375:VAL:HG22	1:B:397:LEU:HB3	1.91	0.53
1:D:65:LEU:HD23	1:D:65:LEU:C	2.34	0.53
1:A:75:MET:HG2	1:A:107:ALA:O	2.08	0.53
1:B:154:GLU:HA	3:B:2007:HOH:O	2.08	0.53
1:C:175:LYS:HD3	1:C:206:HIS:HE1	1.74	0.53
1:D:74:THR:OG1	1:D:156:LYS:HB2	2.09	0.53
1:C:132:MET:HA	1:C:147:LEU:HG	1.91	0.53
1:C:142:VAL:CG1	1:C:143:ILE:N	2.71	0.53
1:C:373:LEU:HA	1:C:394:ALA:HB1	1.91	0.53
1:A:320:TYR:HB3	1:A:323:GLU:HB2	1.90	0.53
1:C:136:ALA:O	1:C:142:VAL:HG13	2.09	0.53
1:A:172:GLU:OE1	1:A:175:LYS:HD2	2.09	0.52
1:C:92:THR:OG1	1:C:143:ILE:CA	2.39	0.52
1:D:284:MET:HA	1:D:287:ASN:O	2.09	0.52
1:A:96:ASP:C	1:A:98:SER:N	2.67	0.52
1:A:299:ALA:HB3	1:C:257:ILE:HD11	1.91	0.52
1:C:96:ASP:O	1:C:98:SER:N	2.43	0.52
1:C:230:PHE:CE1	1:C:263:MET:HG2	2.44	0.52
1:C:434:LYS:CG	1:C:451:MET:CE	2.84	0.52
1:B:452:VAL:CG1	1:B:462:THR:CG2	2.88	0.52
1:C:110:TYR:O	1:C:112:GLY:N	2.43	0.52
1:C:137:ILE:CG1	1:C:142:VAL:HG11	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LYS:HD2	1:D:241:MET:SD	2.49	0.52
1:C:284:MET:HE3	1:C:288:PRO:C	2.35	0.52
1:D:284:MET:HE3	1:D:288:PRO:C	2.34	0.52
1:A:88:GLY:CA	1:A:145:LYS:CE	2.38	0.52
1:B:229:ASN:O	1:B:230:PHE:C	2.53	0.52
1:B:391:PHE:N	1:B:392:PRO:CD	2.73	0.52
1:D:160:LEU:HB2	1:D:165:ILE:HD11	1.91	0.52
1:D:114:THR:HG22	1:D:137:ILE:HG23	1.91	0.52
1:A:118:SER:O	1:A:119:VAL:C	2.52	0.51
1:D:118:SER:O	1:D:121:ASN:HB2	2.08	0.51
1:B:118:SER:O	1:B:119:VAL:C	2.53	0.51
1:C:113:PHE:CD1	1:C:117:LEU:HD23	2.43	0.51
1:C:137:ILE:HG12	1:C:142:VAL:CB	2.41	0.51
1:C:320:TYR:HB3	1:C:323:GLU:HB2	1.91	0.51
1:D:274:VAL:HG22	1:D:275:ILE:N	2.24	0.51
1:A:86:LYS:O	1:A:87:ALA:C	2.53	0.51
1:B:363:VAL:O	1:B:367:GLU:HG3	2.10	0.51
1:C:137:ILE:HG21	1:C:142:VAL:HG22	1.93	0.51
1:A:240:ILE:O	1:A:275:ILE:N	2.38	0.51
1:B:133:GLU:O	1:B:144:CYS:CA	2.59	0.51
1:A:311:LEU:HD22	1:A:314:GLU:HB2	1.93	0.51
1:B:354:ILE:O	1:B:358:VAL:HG23	2.11	0.51
1:C:170:LEU:HD13	1:C:175:LYS:HA	1.93	0.51
1:A:25:ASP:OD1	1:A:59:LYS:NZ	2.32	0.51
1:A:31:MET:HE2	1:A:50:LEU:CD2	2.41	0.51
1:C:118:SER:C	1:C:134:VAL:HG11	2.36	0.51
1:C:172:GLU:HG2	1:C:175:LYS:HZ1	1.76	0.50
1:D:17:GLU:O	1:D:21:ALA:N	2.36	0.50
1:B:80:GLY:CA	1:B:154:GLU:OE2	2.56	0.50
1:B:354:ILE:O	1:B:355:THR:C	2.53	0.50
1:B:387:VAL:CG1	1:B:396:ILE:HD13	2.41	0.50
1:A:15:GLU:HB2	1:A:46:ARG:HG3	1.93	0.50
1:B:10:ILE:HG13	1:B:31:MET:HG3	1.91	0.50
1:B:193:PHE:CE2	1:B:195:ARG:HD3	2.46	0.50
1:C:94:THR:HA	1:C:140:ASN:O	2.12	0.50
1:B:220:LYS:HE2	1:B:222:GLU:OE2	2.12	0.50
1:B:449:VAL:HG11	1:B:451:MET:HE2	1.93	0.50
1:D:133:GLU:O	1:D:144:CYS:HA	2.12	0.50
1:A:64:LEU:C	1:A:64:LEU:HD23	2.37	0.50
1:A:70:PRO:CB	1:A:167:LEU:HD13	2.42	0.50
1:A:88:GLY:HA2	1:A:145:LYS:CD	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:THR:HG21	1:C:302:ILE:HG12	1.94	0.50
1:C:240:ILE:O	1:C:275:ILE:N	2.37	0.50
1:D:191:ALA:CB	1:D:203:ILE:HD13	2.41	0.50
1:D:402:ASN:ND2	1:D:402:ASN:C	2.69	0.50
1:C:167:LEU:HD22	1:C:168:PRO:CD	2.42	0.50
1:C:251:ILE:CB	1:C:252:PRO:CD	2.88	0.50
1:A:436:LEU:O	1:A:440:SER:HB3	2.12	0.50
1:B:9:THR:HG23	1:B:32:ARG:HG2	1.93	0.50
1:C:118:SER:N	1:C:121:ASN:OD1	2.45	0.50
1:D:160:LEU:CB	1:D:163:VAL:HB	2.42	0.50
1:A:440:SER:OG	1:A:442:LEU:HB2	2.12	0.49
1:B:174:ASP:O	1:B:178:LEU:HG	2.12	0.49
1:B:261:LYS:O	1:B:262:MET:C	2.55	0.49
1:C:325:VAL:O	1:C:328:MET:HB3	2.12	0.49
1:A:45:GLN:CG	3:A:2007:HOH:O	2.59	0.49
1:C:74:THR:HA	1:C:108:VAL:HG12	1.93	0.49
1:C:324:ALA:O	1:C:325:VAL:C	2.48	0.49
1:D:334:ARG:HD2	1:D:337:ARG:HH12	1.76	0.49
1:C:50:LEU:HG	1:C:54:MET:CE	2.32	0.49
1:C:195:ARG:NH2	3:C:2014:HOH:O	2.46	0.49
1:D:230:PHE:CZ	1:D:263:MET:HG2	2.46	0.49
1:B:171:ALA:O	1:B:174:ASP:HB2	2.12	0.49
1:C:360:ARG:NH2	1:C:364:GLU:OE1	2.46	0.49
1:D:28:MET:CE	1:D:31:MET:HA	2.43	0.49
1:A:133:GLU:O	1:A:144:CYS:HB3	2.12	0.49
1:A:281:LEU:HB3	1:A:284:MET:HG3	1.93	0.49
1:B:75:MET:HG3	1:B:107:ALA:C	2.37	0.49
1:C:137:ILE:CG2	1:C:141:LYS:O	2.54	0.49
1:B:51:ARG:HA	1:B:54:MET:HE3	1.93	0.49
1:B:409:LEU:O	1:B:410:VAL:C	2.55	0.49
1:D:267:CYS:HB3	1:D:272:LYS:O	2.12	0.49
1:A:132:MET:HG2	1:A:146:VAL:HA	1.94	0.49
1:B:312:SER:N	1:B:314:GLU:OE1	2.44	0.49
1:A:35:PHE:CZ	1:A:43:HIS:CD2	3.01	0.49
1:C:75:MET:HG2	1:C:107:ALA:HB3	1.94	0.49
1:A:402:ASN:HD22	1:A:405:THR:H	1.60	0.49
1:C:130:ILE:CG2	1:C:132:MET:HE1	2.42	0.49
1:D:388:ARG:O	1:D:389:LYS:C	2.56	0.49
1:A:191:ALA:CB	1:A:203:ILE:CD1	2.91	0.48
1:C:10:ILE:HG22	1:C:46:ARG:HD3	1.94	0.48
1:C:92:THR:OG1	1:C:143:ILE:CG1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:CG1	1:D:100:ILE:N	2.76	0.48
1:A:126:ASP:O	1:A:127:ASP:C	2.56	0.48
1:A:299:ALA:HB3	1:C:257:ILE:CD1	2.43	0.48
1:C:119:VAL:CA	1:C:134:VAL:HG11	2.35	0.48
1:C:373:LEU:HD11	1:C:397:LEU:HB2	1.95	0.48
1:D:119:VAL:HG12	1:D:120:GLY:N	2.28	0.48
1:D:320:TYR:HB3	1:D:323:GLU:HB2	1.95	0.48
1:A:402:ASN:C	1:A:402:ASN:ND2	2.64	0.48
1:C:191:ALA:C	1:C:220:LYS:HG3	2.35	0.48
1:A:76:LYS:HA	1:A:154:GLU:OE1	2.13	0.48
1:D:324:ALA:O	1:D:325:VAL:C	2.56	0.48
1:D:440:SER:OG	1:D:442:LEU:HG	2.13	0.48
1:B:123:VAL:HG12	1:B:124:LEU:N	2.29	0.48
1:C:64:LEU:C	1:C:64:LEU:HD23	2.39	0.48
1:C:281:LEU:O	1:C:314:GLU:HG2	2.12	0.48
1:D:327:ILE:O	1:D:331:ILE:HG13	2.14	0.48
1:C:119:VAL:HG22	1:C:134:VAL:HG12	1.96	0.48
1:C:287:ASN:HB3	1:C:288:PRO:HD2	1.95	0.48
1:C:355:THR:HG23	1:C:462:THR:HB	1.96	0.48
1:D:409:LEU:O	1:D:410:VAL:C	2.51	0.48
1:D:281:LEU:HD12	1:D:311:LEU:HD21	1.96	0.48
1:A:96:ASP:OD1	1:A:98:SER:OG	2.24	0.48
1:A:463:ASN:O	1:B:466:SER:HA	2.14	0.48
1:C:175:LYS:HG2	1:C:206:HIS:ND1	2.26	0.48
1:D:84:SER:C	1:D:85:LEU:HD23	2.39	0.48
1:A:19:MET:O	1:A:20:LEU:C	2.57	0.47
1:A:133:GLU:HB2	1:A:147:LEU:CD2	2.43	0.47
1:B:334:ARG:HH11	1:D:255:GLU:CD	2.21	0.47
1:C:15:GLU:O	1:C:16:SER:C	2.53	0.47
1:C:172:GLU:HG2	1:C:175:LYS:NZ	2.30	0.47
1:D:132:MET:HA	1:D:147:LEU:HG	1.96	0.47
1:D:179:ILE:O	1:D:183:GLU:HG3	2.15	0.47
1:B:31:MET:HE2	1:B:63:ILE:HG12	1.96	0.47
1:C:16:SER:O	1:C:20:LEU:HG	2.14	0.47
1:D:171:ALA:O	1:D:174:ASP:HB2	2.14	0.47
1:A:335:THR:O	1:A:336:ASP:C	2.57	0.47
1:A:161:PRO:O	1:A:163:VAL:N	2.48	0.47
1:C:83:VAL:CG2	1:C:103:SER:HA	2.44	0.47
1:C:140:ASN:OD1	1:C:141:LYS:CD	2.62	0.47
1:C:170:LEU:HD11	1:C:178:LEU:HD12	1.96	0.47
1:C:117:LEU:HD12	1:C:121:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLY:C	1:C:240:ILE:HG12	2.40	0.47
1:C:19:MET:O	1:C:20:LEU:C	2.55	0.47
1:A:428:ASP:OD1	1:A:431:ARG:NH1	2.48	0.47
1:B:23:MET:CE	1:B:325:VAL:CG2	2.92	0.47
1:C:335:THR:O	1:C:336:ASP:C	2.56	0.47
1:A:75:MET:HB2	1:A:76:LYS:H	1.46	0.47
1:A:181:GLY:O	1:A:185:GLY:N	2.48	0.47
1:C:126:ASP:O	1:C:127:ASP:C	2.56	0.47
1:A:9:THR:HG23	1:A:32:ARG:HG2	1.96	0.47
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.82	0.47
1:B:154:GLU:O	1:B:155:ASN:HB3	2.14	0.47
1:C:23:MET:HE2	1:C:325:VAL:HG21	1.97	0.47
1:C:84:SER:C	1:C:85:LEU:HD23	2.40	0.47
1:B:96:ASP:O	1:B:98:SER:N	2.49	0.46
1:A:65:LEU:HD23	1:A:65:LEU:C	2.41	0.46
1:A:159:ASN:C	1:A:161:PRO:HD3	2.41	0.46
1:A:466:SER:OG	1:A:468:HIS:NE2	2.42	0.46
1:C:15:GLU:HB2	1:C:46:ARG:HG3	1.97	0.46
1:D:5:LYS:HG3	1:D:410:VAL:O	2.16	0.46
1:B:188:PHE:CD1	1:B:216:HIS:HB2	2.50	0.46
1:B:245:GLY:O	1:B:246:ASP:C	2.57	0.46
1:A:51:ARG:HA	1:A:54:MET:CE	2.29	0.46
1:B:191:ALA:HB2	1:B:203:ILE:CD1	2.45	0.46
1:C:110:TYR:O	1:C:113:PHE:N	2.45	0.46
1:C:191:ALA:HB2	1:C:203:ILE:HD13	1.97	0.46
1:C:341:SER:HA	1:C:391:PHE:O	2.15	0.46
1:A:135:THR:O	1:A:136:ALA:HB2	2.15	0.46
1:A:140:ASN:OD1	1:A:141:LYS:NZ	2.43	0.46
1:C:118:SER:O	1:C:119:VAL:C	2.58	0.46
1:C:119:VAL:CG2	1:C:135:THR:C	2.89	0.46
1:D:354:ILE:O	1:D:355:THR:C	2.58	0.46
1:D:373:LEU:HD12	1:D:395:THR:O	2.16	0.46
1:B:14:THR:HA	1:B:19:MET:HG2	1.97	0.46
1:B:133:GLU:O	1:B:144:CYS:HB3	2.14	0.46
1:C:326:SER:O	1:C:330:THR:HG23	2.16	0.46
1:D:118:SER:O	1:D:119:VAL:C	2.57	0.46
1:B:239:GLY:C	1:B:240:ILE:HG12	2.40	0.46
1:C:74:THR:HG22	1:C:93:PHE:CE1	2.49	0.46
1:C:174:ASP:O	1:C:175:LYS:C	2.59	0.46
1:C:321:PRO:HG2	1:C:322:LEU:H	1.80	0.46
1:C:452:VAL:CG1	1:C:462:THR:CG2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:O	1:D:199:ASP:HB2	2.16	0.46
1:B:258:PHE:HZ	1:D:335:THR:HG23	1.81	0.46
1:C:23:MET:CE	1:C:325:VAL:HG21	2.45	0.46
1:C:159:ASN:ND2	1:C:249:VAL:CG1	2.79	0.46
1:D:363:VAL:O	1:D:367:GLU:HG3	2.16	0.46
1:D:458:PRO:O	1:D:459:SER:C	2.58	0.46
1:D:10:ILE:HG13	1:D:31:MET:SD	2.56	0.45
1:C:202:GLU:HG3	3:C:2016:HOH:O	2.06	0.45
1:A:4:THR:HG21	1:A:302:ILE:HG12	1.98	0.45
1:A:281:LEU:HB2	1:A:314:GLU:HG2	1.97	0.45
1:B:274:VAL:O	1:B:274:VAL:HG13	2.16	0.45
1:B:436:LEU:O	1:B:437:ALA:C	2.58	0.45
1:C:14:THR:CG2	1:C:315:SER:O	2.59	0.45
1:A:88:GLY:C	1:A:145:LYS:HD2	2.41	0.45
1:C:128:GLY:O	1:C:129:LEU:C	2.59	0.45
1:C:140:ASN:OD1	1:C:141:LYS:CE	2.63	0.45
1:C:267:CYS:HB3	1:C:272:LYS:O	2.15	0.45
1:D:19:MET:O	1:D:20:LEU:C	2.59	0.45
1:A:229:ASN:O	1:A:230:PHE:C	2.60	0.45
1:C:320:TYR:N	1:C:321:PRO:CD	2.80	0.45
1:D:152:LEU:HD12	1:D:152:LEU:HA	1.65	0.45
1:D:198:SER:HB3	3:D:2029:HOH:O	2.16	0.45
1:A:75:MET:HE3	1:A:75:MET:HB3	1.66	0.45
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.68	0.45
1:B:428:ASP:OD1	1:B:431:ARG:NH1	2.49	0.45
1:B:440:SER:OG	1:B:442:LEU:HG	2.17	0.45
1:A:440:SER:OG	1:A:442:LEU:HG	2.17	0.45
1:D:271:LEU:O	1:D:385:ARG:HD2	2.17	0.45
1:C:204:ARG:HH22	1:C:238:ASP:CG	2.20	0.45
1:B:449:VAL:CG1	1:B:451:MET:HE2	2.46	0.44
1:C:140:ASN:C	1:C:141:LYS:HG3	2.41	0.44
1:A:203:ILE:HD13	1:A:203:ILE:HG21	1.75	0.44
1:B:402:ASN:ND2	1:B:402:ASN:C	2.73	0.44
1:A:176:GLN:H	1:A:176:GLN:HG3	1.59	0.44
1:A:452:VAL:CG1	1:A:462:THR:CG2	2.95	0.44
1:A:395:THR:CG2	1:A:396:ILE:N	2.80	0.44
1:B:8:CYS:HB2	1:B:28:MET:CE	2.35	0.44
1:B:191:ALA:C	1:B:220:LYS:HG3	2.40	0.44
1:C:110:TYR:C	1:C:112:GLY:N	2.75	0.44
1:D:387:VAL:HG12	1:D:396:ILE:CD1	2.47	0.44
1:D:230:PHE:CD1	1:D:263:MET:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:CB	1:A:174:ASP:OD2	2.66	0.44
1:A:287:ASN:HB3	1:A:288:PRO:CD	2.48	0.44
1:A:354:ILE:O	1:A:355:THR:C	2.60	0.44
1:B:458:PRO:O	1:B:459:SER:C	2.58	0.44
1:C:192:SER:O	1:C:193:PHE:C	2.60	0.44
1:D:388:ARG:HD3	1:D:388:ARG:C	2.42	0.44
1:A:24:LEU:HA	1:A:28:MET:HB3	1.98	0.44
1:A:455:ALA:O	1:A:456:LEU:C	2.61	0.44
1:B:391:PHE:N	1:B:392:PRO:HD2	2.32	0.44
1:C:73:ARG:HA	1:C:73:ARG:HD3	1.85	0.44
1:C:113:PHE:CD1	1:C:117:LEU:HD22	2.50	0.44
1:D:119:VAL:HA	1:D:134:VAL:HG12	2.00	0.44
1:D:320:TYR:N	1:D:321:PRO:CD	2.80	0.44
1:A:76:LYS:HG2	1:A:154:GLU:OE1	2.18	0.44
1:A:124:LEU:O	1:A:158:VAL:HA	2.18	0.44
1:A:320:TYR:N	1:A:321:PRO:CD	2.80	0.44
1:B:452:VAL:CG1	1:B:462:THR:HG21	2.48	0.44
1:C:395:THR:CG2	1:C:396:ILE:N	2.80	0.44
1:D:402:ASN:ND2	1:D:405:THR:N	2.56	0.44
1:C:110:TYR:OH	1:C:116:ASP:OD2	2.36	0.44
1:D:86:LYS:O	1:D:87:ALA:C	2.58	0.44
1:D:99:VAL:HG12	1:D:100:ILE:N	2.33	0.44
1:A:105:MET:CG	1:A:106:VAL:N	2.79	0.43
1:A:191:ALA:HB1	1:A:203:ILE:HD11	1.99	0.43
1:A:426:THR:HG22	1:A:430:TYR:CE2	2.52	0.43
1:C:96:ASP:C	1:C:98:SER:H	2.26	0.43
1:D:131:GLY:C	1:D:132:MET:CG	2.91	0.43
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.88	0.43
1:A:354:ILE:HG21	1:A:354:ILE:HD13	1.76	0.43
1:A:395:THR:HG22	1:A:396:ILE:N	2.32	0.43
1:C:119:VAL:CG2	1:C:134:VAL:HG12	2.48	0.43
1:C:363:VAL:O	1:C:367:GLU:HG3	2.18	0.43
1:D:193:PHE:CE2	1:D:195:ARG:HD3	2.54	0.43
1:B:96:ASP:C	1:B:98:SER:H	2.26	0.43
1:B:159:ASN:CG	1:B:249:VAL:HG11	2.42	0.43
1:D:96:ASP:O	1:D:98:SER:N	2.51	0.43
1:C:188:PHE:CE1	1:C:216:HIS:HB2	2.53	0.43
1:D:165:ILE:HG22	1:D:167:LEU:H	1.82	0.43
1:D:375:VAL:HA	1:D:397:LEU:O	2.18	0.43
1:B:179:ILE:O	1:B:183:GLU:HG3	2.18	0.43
1:B:456:LEU:O	1:B:457:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ASN:ND2	1:C:249:VAL:HG11	2.33	0.43
1:D:117:LEU:HD11	1:D:160:LEU:HD22	2.00	0.43
1:D:131:GLY:C	1:D:132:MET:HG3	2.42	0.43
1:D:174:ASP:O	1:D:178:LEU:HG	2.18	0.43
1:D:227:LEU:HD12	1:D:227:LEU:HA	1.67	0.43
1:D:405:THR:O	1:D:406:ALA:C	2.60	0.43
1:B:160:LEU:HD12	1:B:165:ILE:HD13	2.01	0.43
1:A:10:ILE:HG13	1:A:31:MET:CG	2.44	0.43
1:A:117:LEU:HD21	1:A:123:VAL:HG23	2.00	0.43
1:A:152:LEU:HG	1:A:153:GLY:O	2.18	0.43
1:C:430:TYR:HA	1:C:451:MET:SD	2.58	0.43
1:D:387:VAL:HG12	1:D:396:ILE:HD11	2.00	0.43
1:A:284:MET:C	1:A:286:LYS:N	2.68	0.43
1:B:251:ILE:HB	1:B:252:PRO:CD	2.49	0.43
1:D:14:THR:HA	1:D:19:MET:HG2	2.01	0.43
1:B:86:LYS:O	1:B:87:ALA:C	2.61	0.43
1:B:252:PRO:O	1:B:253:VAL:C	2.62	0.43
1:C:281:LEU:HD12	1:C:311:LEU:HD21	2.00	0.43
1:A:67:THR:CG2	1:A:178:LEU:HD21	2.49	0.43
1:B:23:MET:HE1	1:B:325:VAL:CG2	2.48	0.43
1:C:77:LEU:HD11	1:C:154:GLU:N	2.33	0.43
1:C:171:ALA:O	1:C:172:GLU:C	2.61	0.43
1:A:16:SER:O	1:A:17:GLU:C	2.60	0.42
1:A:204:ARG:HH22	1:A:238:ASP:CG	2.21	0.42
1:B:124:LEU:HD12	1:B:249:VAL:HG13	1.99	0.42
1:C:77:LEU:HD11	1:C:153:GLY:C	2.44	0.42
1:C:193:PHE:CE2	1:C:195:ARG:HD3	2.54	0.42
1:A:10:ILE:HD13	1:A:10:ILE:HA	1.75	0.42
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.75	0.42
1:C:284:MET:C	1:C:286:LYS:N	2.70	0.42
1:C:287:ASN:HB3	1:C:288:PRO:CD	2.48	0.42
1:A:110:TYR:O	1:A:112:GLY:N	2.52	0.42
1:C:171:ALA:O	1:C:173:LYS:N	2.51	0.42
1:D:70:PRO:HB2	1:D:167:LEU:HD13	2.01	0.42
1:A:19:MET:HE1	1:A:322:LEU:HD22	2.01	0.42
1:A:173:LYS:O	1:A:174:ASP:C	2.61	0.42
1:A:23:MET:CE	1:A:325:VAL:CG2	2.97	0.42
1:A:165:ILE:HG22	1:A:167:LEU:H	1.84	0.42
1:C:160:LEU:N	1:C:161:PRO:HD3	2.34	0.42
1:C:171:ALA:O	1:C:174:ASP:N	2.52	0.42
1:C:220:LYS:HB2	1:C:222:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ILE:HB	1:D:252:PRO:CD	2.48	0.42
1:A:160:LEU:HB2	1:A:163:VAL:HB	2.02	0.42
1:A:240:ILE:O	1:A:274:VAL:HA	2.19	0.42
1:C:136:ALA:O	1:C:143:ILE:HB	2.19	0.42
1:C:230:PHE:CZ	1:C:263:MET:HG2	2.53	0.42
1:D:138:GLU:O	1:D:141:LYS:HB2	2.19	0.42
1:D:284:MET:O	1:D:285:ILE:C	2.59	0.42
1:D:434:LYS:CG	1:D:451:MET:HE1	2.32	0.42
1:A:8:CYS:HB2	1:A:28:MET:HE3	2.02	0.42
1:A:94:THR:HA	1:A:140:ASN:O	2.19	0.42
1:A:197:ARG:HB2	1:A:232:GLU:HG3	1.99	0.42
1:A:220:LYS:HB2	1:A:222:GLU:OE2	2.19	0.42
1:B:292:ARG:O	1:B:293:ALA:C	2.59	0.42
1:C:134:VAL:HA	1:C:144:CYS:HB3	2.01	0.42
1:C:136:ALA:C	1:C:137:ILE:HG13	2.44	0.42
1:C:140:ASN:OD1	1:C:140:ASN:N	2.50	0.42
1:D:10:ILE:HG22	1:D:46:ARG:HD3	2.00	0.42
1:A:31:MET:HE2	1:A:63:ILE:HG12	2.01	0.42
1:A:146:VAL:HG12	1:A:148:ASN:H	1.84	0.42
1:A:147:LEU:O	1:A:148:ASN:HB3	2.18	0.42
1:A:188:PHE:CD1	1:A:216:HIS:CB	3.01	0.42
1:A:430:TYR:HA	1:A:451:MET:SD	2.60	0.42
1:B:430:TYR:O	1:B:434:LYS:HG3	2.19	0.42
1:C:75:MET:HG2	1:C:107:ALA:CB	2.48	0.42
1:D:15:GLU:HB2	1:D:46:ARG:HG3	2.01	0.42
1:C:137:ILE:CG1	1:C:142:VAL:HG22	2.34	0.42
1:B:119:VAL:HG22	1:B:135:THR:C	2.45	0.42
1:C:402:ASN:HB3	1:C:405:THR:HB	2.01	0.42
1:D:197:ARG:O	1:D:198:SER:C	2.63	0.42
1:D:391:PHE:N	1:D:392:PRO:HD2	2.33	0.42
1:A:312:SER:O	1:A:313:GLY:C	2.62	0.41
1:A:391:PHE:N	1:A:392:PRO:CD	2.83	0.41
1:B:10:ILE:HD13	1:B:10:ILE:HA	1.79	0.41
1:B:255:GLU:CD	1:D:334:ARG:HH11	2.28	0.41
1:B:373:LEU:HD11	1:B:397:LEU:HB2	2.02	0.41
1:C:110:TYR:O	1:C:111:GLU:C	2.63	0.41
1:C:173:LYS:HG3	1:C:174:ASP:N	2.30	0.41
1:C:341:SER:HB3	1:C:367:GLU:OE2	2.20	0.41
1:D:395:THR:HG22	1:D:396:ILE:N	2.35	0.41
1:B:110:TYR:OH	1:B:116:ASP:OD2	2.38	0.41
1:C:126:ASP:HB3	1:C:129:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:CG	1:A:90:THR:N	2.79	0.41
1:A:163:VAL:O	1:A:165:ILE:CD1	2.68	0.41
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.71	0.41
1:C:93:PHE:N	1:C:142:VAL:O	2.36	0.41
1:C:94:THR:O	1:C:94:THR:HG23	2.19	0.41
1:C:119:VAL:HG21	1:C:135:THR:O	2.21	0.41
1:C:135:THR:OG1	1:C:143:ILE:CG2	2.66	0.41
1:C:331:ILE:HG21	1:C:331:ILE:HD13	1.75	0.41
1:D:126:ASP:CG	1:D:156:LYS:HD2	2.45	0.41
1:B:320:TYR:N	1:B:321:PRO:CD	2.83	0.41
1:D:96:ASP:C	1:D:98:SER:H	2.29	0.41
1:D:271:LEU:HD12	1:D:382:LYS:HE2	2.03	0.41
1:D:280:MET:HG3	1:D:310:MET:O	2.20	0.41
1:A:355:THR:O	1:A:356:GLU:C	2.63	0.41
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.86	0.41
1:C:75:MET:HE3	1:C:75:MET:HB3	1.84	0.41
1:C:140:ASN:OD1	1:C:141:LYS:HD2	2.21	0.41
1:D:283:SER:C	1:D:285:ILE:N	2.79	0.41
1:A:196:LYS:O	1:A:197:ARG:C	2.62	0.41
1:A:257:ILE:O	1:A:261:LYS:HG3	2.20	0.41
1:A:288:PRO:HB3	1:A:320:TYR:CE1	2.54	0.41
1:B:258:PHE:CZ	1:D:335:THR:HA	2.55	0.41
1:B:271:LEU:HD22	1:B:386:ALA:HA	2.03	0.41
1:B:395:THR:HG22	1:B:396:ILE:N	2.34	0.41
1:D:387:VAL:CG1	1:D:396:ILE:HD13	2.50	0.41
1:A:195:ARG:C	1:A:196:LYS:HG2	2.45	0.41
1:A:425:SER:O	1:A:426:THR:C	2.62	0.41
1:B:260:GLN:O	1:B:261:LYS:C	2.63	0.41
1:B:387:VAL:CG1	1:B:396:ILE:CD1	2.98	0.41
1:C:73:ARG:O	1:C:108:VAL:HA	2.20	0.41
1:D:85:LEU:HD23	1:D:85:LEU:N	2.35	0.41
1:D:92:THR:HG22	1:D:93:PHE:N	2.35	0.41
1:A:86:LYS:O	1:A:89:GLN:HB3	2.20	0.41
1:B:137:ILE:HG12	1:B:142:VAL:HG22	2.03	0.41
1:C:110:TYR:O	1:C:113:PHE:HB2	2.21	0.41
1:C:251:ILE:HD11	1:C:256:VAL:HG22	2.02	0.41
1:C:444:HIS:O	1:C:445:LYS:C	2.63	0.41
1:D:3:LYS:N	1:D:336:ASP:OD2	2.48	0.41
1:D:14:THR:HG21	1:D:315:SER:O	2.19	0.41
1:B:17:GLU:O	1:B:18:GLU:C	2.64	0.41
1:B:113:PHE:O	1:B:117:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLY:N	1:B:134:VAL:O	2.47	0.41
1:B:159:ASN:C	1:B:161:PRO:HD3	2.46	0.41
1:B:299:ALA:CB	1:D:257:ILE:HD11	2.48	0.41
1:B:371:ALA:HB1	1:B:448:VAL:O	2.20	0.41
1:B:388:ARG:O	1:B:389:LYS:C	2.61	0.41
1:C:35:PHE:HZ	1:C:180:PHE:CE2	2.38	0.41
1:C:51:ARG:HA	1:C:54:MET:CE	2.35	0.41
1:C:54:MET:HE3	1:C:54:MET:HB2	1.89	0.41
1:C:75:MET:CG	1:C:107:ALA:HB1	2.50	0.41
1:C:84:SER:OG	1:C:151:ASP:CG	2.64	0.41
1:C:85:LEU:HD13	1:C:91:PHE:CD1	2.56	0.41
1:C:213:GLU:H	1:C:213:GLU:HG3	1.12	0.41
1:C:367:GLU:O	1:C:368:LYS:C	2.62	0.41
1:D:94:THR:HA	1:D:140:ASN:O	2.20	0.41
1:A:230:PHE:CE1	1:A:263:MET:HG2	2.56	0.41
1:B:263:MET:O	1:B:264:ILE:C	2.59	0.41
1:C:373:LEU:HD11	1:C:397:LEU:CB	2.51	0.41
1:C:375:VAL:HG22	1:C:397:LEU:HB3	2.03	0.41
1:C:395:THR:HG22	1:C:396:ILE:N	2.34	0.41
1:D:276:THR:HG21	1:D:301:ALA:CB	2.51	0.41
1:A:255:GLU:OE1	1:C:334:ARG:NH1	2.54	0.40
1:C:8:CYS:HB2	1:C:28:MET:HE3	2.03	0.40
1:C:83:VAL:HG23	1:C:85:LEU:HD21	2.02	0.40
1:C:92:THR:HG21	1:C:143:ILE:CD1	2.50	0.40
1:C:391:PHE:N	1:C:392:PRO:CD	2.84	0.40
1:D:191:ALA:HB2	1:D:203:ILE:HD13	2.03	0.40
1:D:452:VAL:CG1	1:D:462:THR:CG2	2.99	0.40
1:B:230:PHE:CE1	1:B:263:MET:HG2	2.56	0.40
1:D:369:LEU:O	1:D:370:ASP:HB2	2.20	0.40
1:A:89:GLN:HG2	1:A:146:VAL:HG23	2.03	0.40
1:B:92:THR:O	1:B:105:MET:HA	2.22	0.40
1:C:188:PHE:HD1	1:C:216:HIS:HB2	1.81	0.40
1:C:197:ARG:HH11	1:C:197:ARG:HD3	1.34	0.40
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.67	0.40
1:A:191:ALA:C	1:A:220:LYS:HG3	2.42	0.40
1:A:194:ILE:HG13	1:A:219:SER:HB3	2.03	0.40
1:B:281:LEU:C	1:B:314:GLU:HG2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:THR:CG2	1:D:18:GLU:OE2[4_446]	1.86	0.34

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/470 (97%)	434 (95%)	19 (4%)	4 (1%)	14	41
1	B	457/470 (97%)	432 (94%)	24 (5%)	1 (0%)	43	72
1	C	457/470 (97%)	430 (94%)	24 (5%)	3 (1%)	18	47
1	D	457/470 (97%)	441 (96%)	15 (3%)	1 (0%)	43	72
All	All	1828/1880 (97%)	1737 (95%)	82 (4%)	9 (0%)	24	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	162	GLY
1	B	97	LYS
1	C	97	LYS
1	C	172	GLU
1	D	97	LYS
1	A	171	ALA
1	A	111	GLU
1	C	111	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	377/389 (97%)	330 (88%)	47 (12%)	4	15
1	B	377/389 (97%)	334 (89%)	43 (11%)	5	19
1	C	377/389 (97%)	315 (84%)	62 (16%)	2	8
1	D	377/389 (97%)	336 (89%)	41 (11%)	6	21
All	All	1508/1556 (97%)	1315 (87%)	193 (13%)	4	15

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	MET
1	A	60	THR
1	A	75	MET
1	A	84	SER
1	A	89	GLN
1	A	92	THR
1	A	100	ILE
1	A	115	THR
1	A	118	SER
1	A	122	THR
1	A	123	VAL
1	A	133	GLU
1	A	137	ILE
1	A	138	GLU
1	A	145	LYS
1	A	147	LEU
1	A	165	ILE
1	A	172	GLU
1	A	196	LYS
1	A	197	ARG
1	A	198	SER
1	A	201	ILE
1	A	204	ARG
1	A	213	GLU
1	A	220	LYS
1	A	244	ARG
1	A	251	ILE
1	A	253	VAL
1	A	257	ILE
1	A	265	GLU
1	A	284	MET
1	A	292	ARG

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Mol	Chain	Res	Type
1	A	327	ILE
1	A	330	THR
1	A	334	ARG
1	A	356	GLU
1	A	360	ARG
1	A	379	GLN
1	A	402	ASN
1	A	404	LYS
1	A	421	LYS
1	A	431	ARG
1	A	440	SER
1	A	449	VAL
1	A	459	SER
1	A	461	THR
1	B	1	MET
1	B	23	MET
1	B	60	THR
1	B	84	SER
1	B	85	LEU
1	B	89	GLN
1	B	97	LYS
1	B	100	ILE
1	B	104	GLU
1	B	111	GLU
1	B	115	THR
1	B	117	LEU
1	B	121	ASN
1	B	133	GLU
1	B	145	LYS
1	B	154	GLU
1	B	173	LYS
1	B	197	ARG
1	B	198	SER
1	B	201	ILE
1	B	204	ARG
1	B	213	GLU
1	B	220	LYS
1	B	244	ARG
1	B	251	ILE
1	B	253	VAL
1	B	257	ILE
1	B	265	GLU

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Mol	Chain	Res	Type
1	B	285	ILE
1	B	292	ARG
1	B	306	THR
1	B	327	ILE
1	B	330	THR
1	B	356	GLU
1	B	360	ARG
1	B	370	ASP
1	B	379	GLN
1	B	402	ASN
1	B	421	LYS
1	B	431	ARG
1	B	449	VAL
1	B	459	SER
1	B	461	THR
1	C	1	MET
1	C	23	MET
1	C	60	THR
1	C	67	THR
1	C	71	GLU
1	C	75	MET
1	C	76	LYS
1	C	77	LEU
1	C	83	VAL
1	C	85	LEU
1	C	90	THR
1	C	92	THR
1	C	97	LYS
1	C	98	SER
1	C	100	ILE
1	C	103	SER
1	C	104	GLU
1	C	111	GLU
1	C	114	THR
1	C	117	LEU
1	C	119	VAL
1	C	132	MET
1	C	134	VAL
1	C	137	ILE
1	C	142	VAL
1	C	143	ILE
1	C	144	CYS

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Mol	Chain	Res	Type
1	C	145	LYS
1	C	147	LEU
1	C	151	ASP
1	C	152	LEU
1	C	160	LEU
1	C	164	SER
1	C	170	LEU
1	C	173	LYS
1	C	174	ASP
1	C	201	ILE
1	C	204	ARG
1	C	213	GLU
1	C	220	LYS
1	C	232	GLU
1	C	237	SER
1	C	244	ARG
1	C	253	VAL
1	C	257	ILE
1	C	265	GLU
1	C	292	ARG
1	C	327	ILE
1	C	330	THR
1	C	356	GLU
1	C	360	ARG
1	C	370	ASP
1	C	379	GLN
1	C	385	ARG
1	C	395	THR
1	C	404	LYS
1	C	421	LYS
1	C	431	ARG
1	C	440	SER
1	C	449	VAL
1	C	459	SER
1	C	461	THR
1	D	1	MET
1	D	23	MET
1	D	60	THR
1	D	73	ARG
1	D	84	SER
1	D	85	LEU
1	D	98	SER

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Mol	Chain	Res	Type
1	D	100	ILE
1	D	105	MET
1	D	111	GLU
1	D	114	THR
1	D	117	LEU
1	D	121	ASN
1	D	146	VAL
1	D	149	ASN
1	D	151	ASP
1	D	154	GLU
1	D	173	LYS
1	D	197	ARG
1	D	201	ILE
1	D	204	ARG
1	D	213	GLU
1	D	220	LYS
1	D	244	ARG
1	D	253	VAL
1	D	257	ILE
1	D	265	GLU
1	D	292	ARG
1	D	327	ILE
1	D	330	THR
1	D	334	ARG
1	D	356	GLU
1	D	360	ARG
1	D	379	GLN
1	D	402	ASN
1	D	404	LYS
1	D	421	LYS
1	D	431	ARG
1	D	449	VAL
1	D	459	SER
1	D	461	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	45	GLN
1	A	48	GLN
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	52	ASN
1	A	155	ASN
1	A	287	ASN
1	A	340	ASN
1	A	402	ASN
1	B	37	HIS
1	B	48	GLN
1	B	52	ASN
1	B	81	ASN
1	B	159	ASN
1	B	176	GLN
1	B	184	GLN
1	B	206	HIS
1	B	402	ASN
1	B	407	HIS
1	C	159	ASN
1	C	206	HIS
1	C	216	HIS
1	C	224	GLN
1	D	121	ASN
1	D	176	GLN
1	D	214	ASN
1	D	216	HIS
1	D	402	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	B	702	-	4,4,4	0.50	0	6,6,6	0.52	0
2	SO4	C	703	-	4,4,4	0.70	0	6,6,6	0.77	0
2	SO4	D	704	-	4,4,4	0.68	0	6,6,6	0.68	0
2	SO4	A	701	-	4,4,4	0.53	0	6,6,6	0.81	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	704	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	461/470 (98%)	0.03	16 (3%) 47 38	5, 18, 50, 75	0
1	B	461/470 (98%)	-0.05	5 (1%) 78 70	5, 13, 37, 73	0
1	C	461/470 (98%)	0.37	60 (13%) 7 6	5, 17, 70, 100	6 (1%)
1	D	461/470 (98%)	-0.15	1 (0%) 91 88	4, 11, 33, 69	0
All	All	1844/1880 (98%)	0.05	82 (4%) 39 31	4, 14, 53, 100	6 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	LEU	6.5
1	C	105	MET	5.2
1	C	36	SER	5.0
1	C	80	GLY	4.8
1	C	96	ASP	4.6
1	C	106	VAL	4.6
1	C	134	VAL	4.5
1	C	82	ASP	4.4
1	C	101	GLY	4.3
1	C	39	ASP	4.2
1	C	102	ASN	4.1
1	C	118	SER	4.1
1	C	104	GLU	4.0
1	C	98	SER	4.0
1	C	138	GLU	3.8
1	C	75	MET	3.7
1	C	79	GLY	3.7
1	C	88	GLY	3.7
1	C	145	LYS	3.7
1	C	83	VAL	3.7
1	C	142	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	35	PHE	3.6
1	C	81	ASN	3.6
1	C	90	THR	3.6
1	C	95	THR	3.6
1	C	38	GLY	3.5
1	C	137	ILE	3.4
1	A	133	GLU	3.4
1	C	119	VAL	3.4
1	A	114	THR	3.3
1	C	146	VAL	3.3
1	C	171	ALA	3.3
1	A	134	VAL	3.1
1	C	143	ILE	3.1
1	C	87	ALA	3.0
1	C	107	ALA	3.0
1	C	286	LYS	3.0
1	A	135	THR	2.9
1	C	100	ILE	2.9
1	C	120	GLY	2.9
1	C	103	SER	2.8
1	C	78	GLU	2.8
1	C	136	ALA	2.8
1	A	118	SER	2.7
1	C	135	THR	2.7
1	B	356	GLU	2.7
1	C	121	ASN	2.7
1	C	37	HIS	2.6
1	C	141	LYS	2.6
1	B	12	PRO	2.6
1	C	176	GLN	2.6
1	C	147	LEU	2.5
1	C	99	VAL	2.5
1	A	176	GLN	2.5
1	A	344	GLU	2.4
1	C	68	LYS	2.4
1	C	89	GLN	2.4
1	C	97	LYS	2.3
1	C	108	VAL	2.3
1	C	149	ASN	2.3
1	C	69	GLY	2.3
1	A	111	GLU	2.3
1	A	136	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	153	GLY	2.3
1	A	164	SER	2.3
1	A	171	ALA	2.3
1	C	356	GLU	2.3
1	C	76	LYS	2.2
1	C	41	ALA	2.2
1	A	119	VAL	2.2
1	A	78	GLU	2.2
1	C	92	THR	2.2
1	A	120	GLY	2.2
1	A	137	ILE	2.1
1	C	224	GLN	2.1
1	C	93	PHE	2.1
1	B	52	ASN	2.1
1	C	155	ASN	2.1
1	B	39	ASP	2.1
1	A	162	GLY	2.0
1	B	57	THR	2.0
1	D	265	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	704	5/5	0.96	0.10	44,44,45,46	0
2	SO4	B	702	5/5	0.97	0.09	18,19,20,20	0
2	SO4	A	701	5/5	0.97	0.08	21,22,23,23	0
2	SO4	C	703	5/5	0.98	0.06	10,11,12,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.