



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 1LDB / pdb_00001ldb
Title : STRUCTURE DETERMINATION AND REFINEMENT OF BACILLUS
STEARTHERMOPHILUS LACTATE DEHYDROGENASE
Authors : Piontek, K.; Rossmann, M.G.
Deposited on : 1989-03-27
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

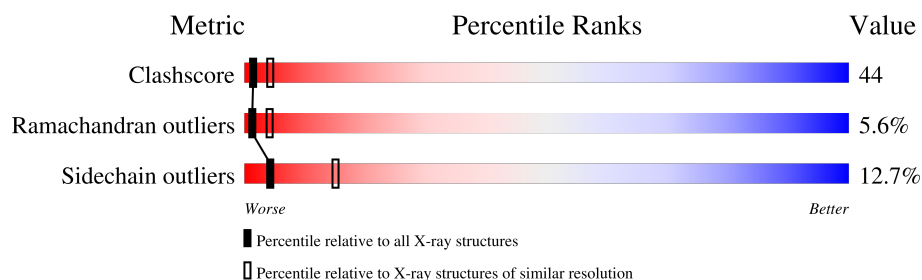
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	16% 35% 32% 10% 7%
1	B	317	15% 34% 33% 10% 7%
1	C	317	16% 33% 33% 10% 7%
1	D	317	15% 33% 33% 11% 7%

2 Entry composition [i](#)

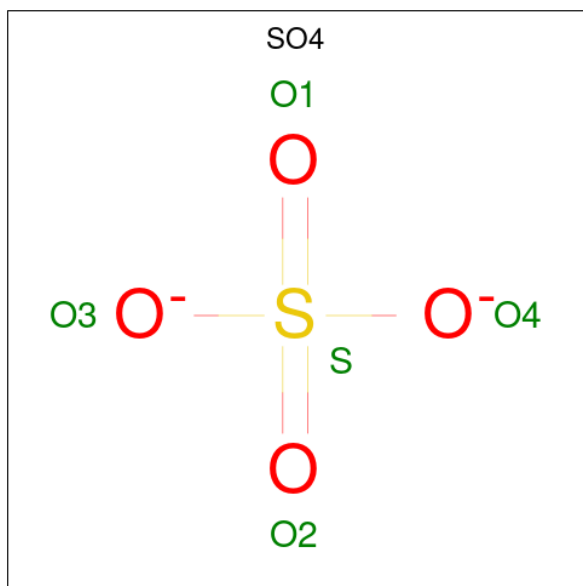
There are 3 unique types of molecules in this entry. The entry contains 9119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APO-L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	B	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	C	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	D	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			

- 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	A	1	Total	O	S	0	0
			5	4	1		

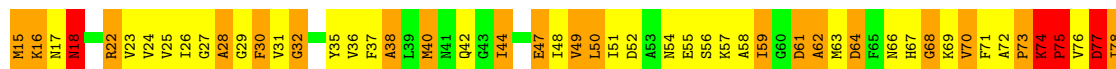
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

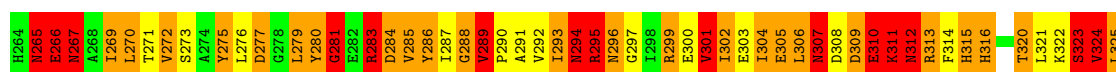
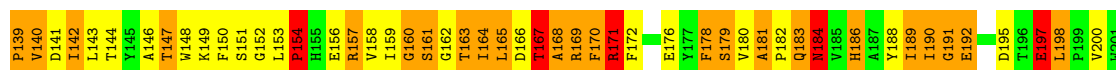
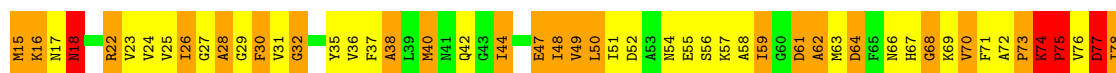




• Molecule 1: APO-L-LACTATE DEHYDROGENASE



• Molecule 1: APO-L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	86.90Å 86.90Å 357.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.286 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9119	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.05	62/2320 (2.7%)	3.16	308/3146 (9.8%)
1	B	2.05	64/2320 (2.8%)	3.16	313/3146 (9.9%)
1	C	2.05	62/2320 (2.7%)	3.16	317/3146 (10.1%)
1	D	2.05	65/2320 (2.8%)	3.16	313/3146 (9.9%)
All	All	2.05	253/9280 (2.7%)	3.16	1251/12584 (9.9%)

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	31
1	B	0	32
1	C	0	31
1	D	0	31
All	All	0	125

All (253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	ILE	C-O	10.43	1.35	1.23
1	A	44	ILE	C-O	10.33	1.35	1.23
1	C	44	ILE	C-O	10.27	1.35	1.23
1	B	44	ILE	C-O	10.20	1.34	1.23
1	C	134	LEU	N-CA	9.98	1.58	1.46
1	D	134	LEU	N-CA	9.92	1.58	1.46
1	A	134	LEU	N-CA	9.92	1.58	1.46
1	B	134	LEU	N-CA	9.89	1.58	1.46
1	C	30	PHE	C-O	8.48	1.33	1.24
1	B	30	PHE	C-O	8.47	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	30	PHE	C-O	8.36	1.33	1.24
1	A	30	PHE	C-O	8.32	1.33	1.24
1	A	161	SER	C-O	-7.95	1.14	1.24
1	B	161	SER	C-O	-7.92	1.14	1.24
1	D	161	SER	C-O	-7.91	1.14	1.24
1	A	280	TYR	N-CA	7.83	1.56	1.46
1	A	52	ASP	N-CA	7.82	1.55	1.45
1	A	138	ASN	N-CA	7.81	1.56	1.45
1	C	138	ASN	N-CA	7.79	1.56	1.45
1	C	161	SER	C-O	-7.78	1.14	1.24
1	B	138	ASN	N-CA	7.77	1.56	1.45
1	C	280	TYR	N-CA	7.77	1.56	1.46
1	D	280	TYR	N-CA	7.75	1.56	1.46
1	B	52	ASP	N-CA	7.73	1.55	1.45
1	B	280	TYR	N-CA	7.73	1.56	1.46
1	D	52	ASP	N-CA	7.72	1.55	1.45
1	D	138	ASN	N-CA	7.71	1.56	1.45
1	B	326	ALA	N-CA	7.66	1.56	1.46
1	C	52	ASP	N-CA	7.61	1.55	1.45
1	C	326	ALA	N-CA	7.60	1.55	1.46
1	A	283	ARG	C-O	7.58	1.34	1.24
1	A	326	ALA	N-CA	7.52	1.55	1.46
1	D	283	ARG	C-O	7.51	1.34	1.24
1	C	283	ARG	C-O	7.50	1.34	1.24
1	D	326	ALA	N-CA	7.50	1.55	1.46
1	B	283	ARG	C-O	7.47	1.34	1.24
1	D	141	ASP	N-CA	7.28	1.55	1.46
1	C	141	ASP	N-CA	7.17	1.55	1.46
1	B	141	ASP	N-CA	7.13	1.55	1.46
1	C	254	GLY	C-O	7.13	1.32	1.23
1	D	254	GLY	C-O	7.13	1.32	1.23
1	A	254	GLY	C-O	7.12	1.32	1.23
1	C	158	VAL	C-O	7.10	1.32	1.24
1	A	141	ASP	N-CA	7.10	1.55	1.46
1	B	158	VAL	C-O	7.05	1.32	1.24
1	A	158	VAL	C-O	7.04	1.31	1.24
1	D	158	VAL	C-O	7.04	1.31	1.24
1	B	277	ASP	CA-CB	7.02	1.65	1.53
1	A	197	GLU	C-O	7.00	1.32	1.23
1	C	277	ASP	CA-CB	7.00	1.65	1.53
1	B	254	GLY	C-O	6.99	1.32	1.23
1	A	277	ASP	CA-CB	6.97	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	197	GLU	C-O	6.95	1.32	1.23
1	B	197	GLU	C-O	6.94	1.32	1.23
1	D	277	ASP	CA-CB	6.90	1.65	1.53
1	C	197	GLU	C-O	6.86	1.32	1.23
1	D	16	LYS	N-CA	6.82	1.50	1.46
1	C	163	THR	C-O	6.75	1.33	1.24
1	B	163	THR	C-O	6.67	1.32	1.24
1	A	163	THR	C-O	6.63	1.32	1.24
1	D	163	THR	C-O	6.59	1.32	1.24
1	B	281	GLY	N-CA	6.58	1.54	1.45
1	A	281	GLY	N-CA	6.52	1.54	1.45
1	C	281	GLY	N-CA	6.51	1.54	1.45
1	A	119	SER	N-CA	6.51	1.54	1.46
1	C	16	LYS	N-CA	6.50	1.50	1.46
1	B	16	LYS	N-CA	6.50	1.50	1.46
1	A	16	LYS	N-CA	6.47	1.50	1.46
1	B	119	SER	N-CA	6.44	1.54	1.46
1	C	119	SER	N-CA	6.42	1.54	1.46
1	A	261	ALA	C-N	-6.41	1.25	1.33
1	D	281	GLY	N-CA	6.40	1.53	1.45
1	D	119	SER	N-CA	6.38	1.54	1.46
1	B	279	LEU	C-N	-6.38	1.24	1.33
1	B	76	VAL	C-N	-6.37	1.24	1.33
1	B	261	ALA	C-N	-6.35	1.26	1.33
1	A	76	VAL	C-N	-6.35	1.24	1.33
1	C	277	ASP	N-CA	-6.34	1.37	1.46
1	C	76	VAL	C-N	-6.33	1.24	1.33
1	C	160	GLY	CA-C	6.33	1.57	1.51
1	B	277	ASP	N-CA	-6.33	1.37	1.46
1	B	160	GLY	CA-C	6.33	1.57	1.51
1	A	279	LEU	C-N	-6.32	1.24	1.33
1	D	261	ALA	C-N	-6.31	1.26	1.33
1	C	279	LEU	C-N	-6.30	1.24	1.33
1	D	279	LEU	C-N	-6.30	1.24	1.33
1	D	76	VAL	C-N	-6.29	1.24	1.33
1	A	160	GLY	CA-C	6.25	1.57	1.51
1	A	277	ASP	N-CA	-6.24	1.38	1.46
1	A	74	LYS	CA-CB	6.23	1.63	1.53
1	D	160	GLY	CA-C	6.23	1.57	1.51
1	C	261	ALA	C-N	-6.19	1.26	1.33
1	D	277	ASP	N-CA	-6.17	1.38	1.46
1	D	74	LYS	CA-CB	6.17	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	ALA	CA-CB	-6.15	1.43	1.53
1	B	74	LYS	CA-CB	6.15	1.63	1.53
1	A	62	ALA	CA-CB	-6.15	1.43	1.53
1	B	62	ALA	CA-CB	-6.14	1.43	1.53
1	D	62	ALA	CA-CB	-6.14	1.43	1.53
1	C	74	LYS	CA-CB	6.11	1.63	1.53
1	B	308	ASP	N-CA	6.09	1.53	1.46
1	C	226	LEU	N-CA	-6.07	1.38	1.46
1	D	226	LEU	N-CA	-6.05	1.38	1.46
1	C	308	ASP	N-CA	5.99	1.53	1.46
1	B	226	LEU	N-CA	-5.99	1.38	1.46
1	D	141	ASP	CA-CB	-5.99	1.43	1.53
1	B	141	ASP	CA-CB	-5.98	1.43	1.53
1	C	279	LEU	CA-CB	-5.97	1.44	1.53
1	A	141	ASP	CA-CB	-5.97	1.43	1.53
1	C	141	ASP	CA-CB	-5.96	1.43	1.53
1	D	279	LEU	CA-CB	-5.93	1.44	1.53
1	A	279	LEU	CA-CB	-5.92	1.44	1.53
1	A	226	LEU	N-CA	-5.91	1.38	1.46
1	D	136	ALA	C-N	-5.90	1.25	1.33
1	A	136	ALA	C-N	-5.89	1.25	1.33
1	D	308	ASP	N-CA	5.88	1.53	1.46
1	B	126	ALA	C-O	5.87	1.31	1.24
1	A	308	ASP	N-CA	5.87	1.53	1.46
1	B	279	LEU	CA-CB	-5.84	1.44	1.53
1	A	126	ALA	C-O	5.84	1.31	1.24
1	D	139	PRO	C-N	-5.83	1.26	1.33
1	D	126	ALA	C-O	5.83	1.31	1.24
1	B	136	ALA	C-N	-5.81	1.25	1.33
1	C	136	ALA	C-N	-5.81	1.25	1.33
1	B	190	ILE	N-CA	5.80	1.53	1.46
1	C	126	ALA	C-O	5.80	1.31	1.24
1	B	139	PRO	C-N	-5.80	1.26	1.33
1	C	137	THR	CA-CB	5.79	1.61	1.53
1	C	52	ASP	C-O	5.78	1.30	1.23
1	D	52	ASP	C-O	5.77	1.30	1.23
1	A	52	ASP	C-O	5.77	1.30	1.23
1	A	139	PRO	C-N	-5.76	1.26	1.33
1	A	190	ILE	N-CA	5.76	1.53	1.46
1	C	190	ILE	N-CA	5.75	1.53	1.46
1	D	190	ILE	N-CA	5.74	1.53	1.46
1	D	168	ALA	C-O	-5.74	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	ASP	C-O	5.74	1.30	1.23
1	C	67	HIS	ND1-CE1	5.72	1.38	1.32
1	D	137	THR	CA-CB	5.72	1.60	1.53
1	A	168	ALA	C-O	-5.70	1.17	1.24
1	B	137	THR	CA-CB	5.70	1.60	1.53
1	C	25	VAL	C-N	-5.69	1.26	1.33
1	B	67	HIS	ND1-CE1	5.69	1.38	1.32
1	C	139	PRO	C-N	-5.67	1.26	1.33
1	B	168	ALA	C-O	-5.67	1.17	1.24
1	A	137	THR	CA-CB	5.66	1.60	1.53
1	C	168	ALA	C-O	-5.65	1.17	1.24
1	A	25	VAL	C-N	-5.63	1.26	1.33
1	D	25	VAL	C-N	-5.62	1.26	1.33
1	D	67	HIS	ND1-CE1	5.62	1.38	1.32
1	A	123	SER	C-N	-5.62	1.27	1.33
1	D	123	SER	C-N	-5.61	1.27	1.33
1	B	123	SER	C-N	-5.61	1.27	1.33
1	D	284	ASP	C-N	-5.57	1.30	1.33
1	A	67	HIS	ND1-CE1	5.56	1.38	1.32
1	C	164	ILE	C-N	-5.56	1.25	1.33
1	B	159	ILE	C-N	-5.55	1.24	1.32
1	B	25	VAL	C-N	-5.54	1.27	1.33
1	C	159	ILE	C-N	-5.54	1.24	1.32
1	B	164	ILE	C-N	-5.53	1.25	1.33
1	D	159	ILE	C-N	-5.53	1.24	1.32
1	A	29	GLY	C-O	5.53	1.31	1.23
1	C	123	SER	C-N	-5.50	1.27	1.33
1	B	29	GLY	C-O	5.50	1.31	1.23
1	D	164	ILE	C-N	-5.48	1.25	1.33
1	A	159	ILE	C-N	-5.48	1.25	1.32
1	D	30	PHE	C-N	-5.46	1.26	1.33
1	A	164	ILE	C-N	-5.46	1.25	1.33
1	D	292	VAL	C-O	5.45	1.30	1.24
1	A	292	VAL	C-O	5.44	1.30	1.24
1	D	167	THR	C-O	-5.44	1.16	1.24
1	B	167	THR	C-O	-5.44	1.16	1.24
1	A	284	ASP	C-N	-5.43	1.30	1.33
1	C	29	GLY	C-O	5.43	1.31	1.23
1	B	292	VAL	C-O	5.43	1.30	1.24
1	C	292	VAL	C-O	5.41	1.30	1.24
1	A	167	THR	C-O	-5.40	1.16	1.24
1	C	279	LEU	C-O	5.40	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	PHE	C-N	-5.40	1.27	1.33
1	D	29	GLY	C-O	5.40	1.31	1.23
1	B	30	PHE	C-N	-5.40	1.27	1.33
1	C	30	PHE	C-N	-5.40	1.27	1.33
1	C	167	THR	C-O	-5.36	1.17	1.24
1	D	162	GLY	C-O	5.36	1.31	1.24
1	D	279	LEU	C-O	5.36	1.30	1.23
1	C	227	GLU	N-CA	5.35	1.53	1.46
1	C	111	ASP	N-CA	5.35	1.52	1.46
1	B	279	LEU	C-O	5.32	1.30	1.23
1	B	111	ASP	N-CA	5.32	1.52	1.46
1	A	111	ASP	N-CA	5.32	1.52	1.46
1	D	77	ASP	C-N	-5.31	1.27	1.33
1	C	284	ASP	C-N	-5.29	1.30	1.33
1	A	162	GLY	C-O	5.28	1.31	1.24
1	C	162	GLY	C-O	5.28	1.31	1.24
1	A	171	ARG	NE-CZ	5.27	1.38	1.33
1	C	160	GLY	N-CA	-5.27	1.40	1.45
1	B	227	GLU	N-CA	5.27	1.53	1.46
1	A	77	ASP	C-N	-5.26	1.27	1.33
1	A	279	LEU	C-O	5.26	1.30	1.23
1	A	227	GLU	N-CA	5.25	1.52	1.46
1	B	162	GLY	C-O	5.24	1.31	1.24
1	B	284	ASP	C-N	-5.23	1.30	1.33
1	D	271	THR	C-O	5.23	1.29	1.23
1	A	286	TYR	C-N	-5.23	1.26	1.33
1	D	286	TYR	C-N	-5.21	1.26	1.33
1	D	111	ASP	N-CA	5.21	1.52	1.46
1	B	66	ASN	C-O	5.21	1.30	1.24
1	C	77	ASP	C-N	-5.20	1.27	1.33
1	B	77	ASP	C-N	-5.19	1.27	1.33
1	A	66	ASN	C-O	5.18	1.30	1.24
1	C	320	THR	C-O	5.18	1.30	1.24
1	D	227	GLU	N-CA	5.16	1.52	1.46
1	B	160	GLY	N-CA	-5.16	1.40	1.45
1	A	147	THR	N-CA	5.16	1.52	1.46
1	C	271	THR	C-O	5.16	1.29	1.23
1	D	320	THR	C-O	5.15	1.30	1.24
1	B	286	TYR	C-N	-5.14	1.26	1.33
1	A	160	GLY	N-CA	-5.13	1.40	1.45
1	A	271	THR	C-O	5.13	1.29	1.23
1	C	157	ARG	CD-NE	-5.12	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	THR	C-O	5.12	1.29	1.23
1	B	245	GLY	C-O	5.12	1.30	1.23
1	D	171	ARG	NE-CZ	5.12	1.38	1.33
1	D	66	ASN	C-O	5.11	1.30	1.24
1	C	66	ASN	C-O	5.10	1.30	1.24
1	B	147	THR	N-CA	5.10	1.52	1.46
1	B	171	ARG	NE-CZ	5.10	1.38	1.33
1	D	202	SER	C-O	5.09	1.30	1.24
1	B	271	THR	N-CA	5.09	1.53	1.46
1	B	320	THR	C-O	5.09	1.30	1.24
1	C	286	TYR	C-N	-5.09	1.26	1.33
1	B	157	ARG	CD-NE	-5.09	1.39	1.46
1	C	171	ARG	NE-CZ	5.08	1.38	1.33
1	D	160	GLY	N-CA	-5.08	1.40	1.45
1	C	29	GLY	C-N	-5.08	1.27	1.33
1	D	183	GLN	C-N	-5.08	1.26	1.33
1	A	320	THR	C-O	5.07	1.30	1.24
1	D	147	THR	N-CA	5.07	1.52	1.46
1	A	183	GLN	C-N	-5.05	1.26	1.33
1	C	183	GLN	C-N	-5.05	1.26	1.33
1	D	245	GLY	C-O	5.04	1.30	1.23
1	A	171	ARG	C-N	-5.03	1.26	1.33
1	B	183	GLN	C-N	-5.03	1.26	1.33
1	D	29	GLY	C-N	-5.02	1.27	1.33
1	C	202	SER	C-O	5.02	1.30	1.24
1	D	157	ARG	CD-NE	-5.02	1.39	1.46
1	B	29	GLY	C-N	-5.02	1.27	1.33
1	A	271	THR	N-CA	5.01	1.53	1.46
1	C	147	THR	N-CA	5.01	1.52	1.46
1	D	131	GLY	CA-C	-5.01	1.44	1.51
1	B	291	ALA	C-O	5.01	1.30	1.23
1	A	157	ARG	CD-NE	-5.00	1.39	1.46
1	D	271	THR	N-CA	5.00	1.53	1.46

All (1251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	LEU	CA-C-N	22.07	157.57	120.72
1	A	276	LEU	C-N-CA	22.07	157.57	120.72
1	D	276	LEU	CA-C-N	22.06	157.57	120.72
1	D	276	LEU	C-N-CA	22.06	157.57	120.72
1	C	276	LEU	CA-C-N	22.05	157.54	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	LEU	C-N-CA	22.05	157.54	120.72
1	B	276	LEU	CA-C-N	22.03	157.51	120.72
1	B	276	LEU	C-N-CA	22.03	157.51	120.72
1	B	309	ASP	CA-CB-CG	21.95	134.55	112.60
1	C	309	ASP	CA-CB-CG	21.83	134.43	112.60
1	A	309	ASP	CA-CB-CG	21.79	134.39	112.60
1	D	309	ASP	CA-CB-CG	21.72	134.32	112.60
1	C	308	ASP	CA-CB-CG	18.19	130.79	112.60
1	D	308	ASP	CA-CB-CG	18.15	130.75	112.60
1	B	308	ASP	CA-CB-CG	18.09	130.69	112.60
1	A	308	ASP	CA-CB-CG	18.07	130.67	112.60
1	A	169	ARG	NE-CZ-NH1	16.42	137.92	121.50
1	B	169	ARG	NE-CZ-NH1	16.40	137.90	121.50
1	D	169	ARG	NE-CZ-NH1	16.36	137.86	121.50
1	C	169	ARG	NE-CZ-NH1	16.34	137.84	121.50
1	A	159	ILE	CA-C-N	14.67	131.62	121.65
1	A	159	ILE	C-N-CA	14.67	131.62	121.65
1	B	159	ILE	CA-C-N	14.66	131.62	121.65
1	B	159	ILE	C-N-CA	14.66	131.62	121.65
1	D	159	ILE	CA-C-N	14.57	131.56	121.65
1	D	159	ILE	C-N-CA	14.57	131.56	121.65
1	C	159	ILE	CA-C-N	14.54	131.53	121.65
1	C	159	ILE	C-N-CA	14.54	131.53	121.65
1	C	140	VAL	N-CA-C	14.17	124.03	110.42
1	D	140	VAL	N-CA-C	14.16	124.01	110.42
1	A	140	VAL	N-CA-C	14.09	123.95	110.42
1	C	260	ARG	NE-CZ-NH1	-13.32	108.17	121.50
1	B	260	ARG	NE-CZ-NH1	-13.28	108.22	121.50
1	D	260	ARG	NE-CZ-NH1	-13.28	108.22	121.50
1	A	260	ARG	NE-CZ-NH1	-13.21	108.29	121.50
1	D	276	LEU	O-C-N	-13.09	108.08	123.13
1	A	276	LEU	O-C-N	-13.07	108.10	123.13
1	C	276	LEU	O-C-N	-13.06	108.11	123.13
1	B	276	LEU	O-C-N	-13.05	108.13	123.13
1	B	111	ASP	CA-CB-CG	12.95	125.55	112.60
1	B	140	VAL	N-CA-C	12.93	123.94	110.36
1	A	111	ASP	CA-CB-CG	12.92	125.52	112.60
1	C	111	ASP	CA-CB-CG	12.90	125.50	112.60
1	D	111	ASP	CA-CB-CG	12.87	125.47	112.60
1	D	281	GLY	CA-C-O	-12.33	104.98	119.03
1	A	281	GLY	CA-C-O	-12.26	105.05	119.03
1	C	281	GLY	CA-C-O	-12.25	105.06	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	GLY	CA-C-O	-12.23	105.09	119.03
1	B	228	ARG	CD-NE-CZ	-12.16	107.38	124.40
1	C	228	ARG	CD-NE-CZ	-12.15	107.39	124.40
1	D	228	ARG	CD-NE-CZ	-12.15	107.39	124.40
1	A	228	ARG	CD-NE-CZ	-12.13	107.41	124.40
1	A	171	ARG	NE-CZ-NH1	-11.69	109.81	121.50
1	B	171	ARG	NE-CZ-NH1	-11.67	109.83	121.50
1	C	171	ARG	NE-CZ-NH1	-11.67	109.83	121.50
1	D	171	ARG	NE-CZ-NH1	-11.60	109.90	121.50
1	C	169	ARG	CD-NE-CZ	11.30	140.22	124.40
1	B	169	ARG	CD-NE-CZ	11.28	140.20	124.40
1	A	169	ARG	CD-NE-CZ	11.26	140.16	124.40
1	D	169	ARG	CD-NE-CZ	11.26	140.16	124.40
1	B	69	LYS	CA-CB-CG	11.21	136.52	114.10
1	D	69	LYS	CA-CB-CG	11.21	136.53	114.10
1	A	69	LYS	CA-CB-CG	11.20	136.50	114.10
1	C	69	LYS	CA-CB-CG	11.16	136.41	114.10
1	A	74	LYS	N-CA-C	10.80	133.68	109.81
1	C	74	LYS	N-CA-C	10.80	133.68	109.81
1	D	74	LYS	N-CA-C	10.79	133.65	109.81
1	B	74	LYS	N-CA-C	10.78	133.64	109.81
1	C	315	HIS	CA-C-O	10.72	131.78	120.42
1	B	315	HIS	CA-C-O	10.68	131.74	120.42
1	A	315	HIS	CA-C-O	10.66	131.72	120.42
1	C	276	LEU	CA-C-O	10.66	132.37	120.43
1	B	276	LEU	CA-C-O	10.65	132.35	120.43
1	D	315	HIS	CA-C-O	10.64	131.70	120.42
1	A	276	LEU	CA-C-O	10.64	132.35	120.43
1	D	276	LEU	CA-C-O	10.58	132.28	120.43
1	D	228	ARG	NE-CZ-NH1	-10.56	110.94	121.50
1	A	228	ARG	NE-CZ-NH1	-10.53	110.97	121.50
1	C	228	ARG	NE-CZ-NH1	-10.52	110.98	121.50
1	B	228	ARG	NE-CZ-NH1	-10.50	111.00	121.50
1	C	307	ASN	OD1-CG-ND2	10.39	132.99	122.60
1	B	307	ASN	OD1-CG-ND2	10.33	132.93	122.60
1	C	111	ASP	N-CA-CB	10.32	126.08	110.70
1	A	307	ASN	OD1-CG-ND2	10.31	132.91	122.60
1	B	111	ASP	N-CA-CB	10.31	126.06	110.70
1	D	307	ASN	OD1-CG-ND2	10.31	132.91	122.60
1	D	111	ASP	N-CA-CB	10.30	126.04	110.70
1	A	111	ASP	N-CA-CB	10.28	126.02	110.70
1	D	310	GLU	CA-CB-CG	10.20	134.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	GLU	CA-CB-CG	10.18	134.46	114.10
1	C	310	GLU	CA-CB-CG	10.18	134.45	114.10
1	B	310	GLU	CA-CB-CG	10.14	134.39	114.10
1	B	308	ASP	N-CA-C	-10.00	98.64	112.25
1	A	308	ASP	N-CA-C	-10.00	98.65	112.25
1	D	308	ASP	N-CA-C	-9.99	98.66	112.25
1	C	308	ASP	N-CA-C	-9.97	98.69	112.25
1	D	308	ASP	CB-CA-C	9.82	124.79	111.14
1	C	308	ASP	CB-CA-C	9.81	124.77	111.14
1	B	308	ASP	CB-CA-C	9.79	124.74	111.14
1	D	47	GLU	CA-C-O	-9.73	110.00	120.80
1	A	308	ASP	CB-CA-C	9.71	124.64	111.14
1	B	47	GLU	CA-C-O	-9.67	110.06	120.80
1	C	28	ALA	CA-C-O	-9.67	110.75	121.58
1	A	47	GLU	CA-C-O	-9.66	110.08	120.80
1	C	47	GLU	CA-C-O	-9.64	110.10	120.80
1	A	28	ALA	CA-C-O	-9.63	110.79	121.58
1	D	28	ALA	CA-C-O	-9.63	110.79	121.58
1	D	285	VAL	CA-C-O	-9.63	114.21	120.66
1	B	28	ALA	CA-C-O	-9.61	110.81	121.58
1	A	285	VAL	CA-C-O	-9.58	114.24	120.66
1	B	289	VAL	N-CA-CB	-9.57	97.81	111.21
1	A	291	ALA	CA-C-O	-9.56	110.26	121.44
1	C	289	VAL	N-CA-CB	-9.56	97.83	111.21
1	B	285	VAL	CA-C-O	-9.52	114.28	120.66
1	A	289	VAL	N-CA-CB	-9.52	97.88	111.21
1	D	291	ALA	CA-C-O	-9.51	110.31	121.44
1	D	289	VAL	N-CA-CB	-9.50	97.92	111.21
1	C	169	ARG	NH1-CZ-NH2	-9.49	106.96	119.30
1	C	285	VAL	CA-C-O	-9.48	114.31	120.66
1	B	291	ALA	CA-C-O	-9.48	110.35	121.44
1	C	291	ALA	CA-C-O	-9.48	110.35	121.44
1	A	169	ARG	NH1-CZ-NH2	-9.47	106.99	119.30
1	B	169	ARG	NH1-CZ-NH2	-9.46	107.01	119.30
1	D	169	ARG	NH1-CZ-NH2	-9.45	107.02	119.30
1	A	16	LYS	O-C-N	9.43	128.54	121.47
1	A	184	ASN	CB-CG-ND2	9.41	130.51	116.40
1	B	16	LYS	O-C-N	9.40	128.52	121.47
1	A	37	PHE	CA-CB-CG	9.39	123.19	113.80
1	D	294	ASN	CA-CB-CG	9.39	122.00	112.60
1	C	184	ASN	CB-CG-ND2	9.38	130.47	116.40
1	D	37	PHE	CA-CB-CG	9.38	123.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ASN	CB-CG-ND2	9.37	130.45	116.40
1	D	184	ASN	CB-CG-ND2	9.36	130.44	116.40
1	A	294	ASN	CA-CB-CG	9.35	121.95	112.60
1	D	16	LYS	O-C-N	9.33	128.47	121.47
1	C	37	PHE	CA-CB-CG	9.31	123.11	113.80
1	B	37	PHE	CA-CB-CG	9.30	123.10	113.80
1	C	16	LYS	O-C-N	9.29	128.44	121.47
1	B	294	ASN	CA-CB-CG	9.28	121.88	112.60
1	C	294	ASN	CA-CB-CG	9.28	121.88	112.60
1	C	136	ALA	CA-C-O	-9.12	108.68	119.35
1	B	136	ALA	CA-C-O	-9.11	108.69	119.35
1	D	136	ALA	CA-C-O	-9.09	108.71	119.35
1	A	136	ALA	CA-C-O	-9.05	108.76	119.35
1	A	279	LEU	CA-C-O	-9.01	107.09	120.42
1	B	279	LEU	CA-C-O	-9.00	107.10	120.42
1	D	279	LEU	CA-C-O	-9.00	107.11	120.42
1	B	76	VAL	CA-C-N	8.96	136.88	122.81
1	B	76	VAL	C-N-CA	8.96	136.88	122.81
1	C	279	LEU	CA-C-O	-8.95	107.17	120.42
1	A	125	MET	CG-SD-CE	8.95	120.59	100.90
1	D	76	VAL	CA-C-N	8.95	136.86	122.81
1	D	76	VAL	C-N-CA	8.95	136.86	122.81
1	D	125	MET	CG-SD-CE	8.94	120.57	100.90
1	B	125	MET	CG-SD-CE	8.93	120.56	100.90
1	C	125	MET	CG-SD-CE	8.93	120.54	100.90
1	A	76	VAL	CA-C-N	8.92	136.81	122.81
1	A	76	VAL	C-N-CA	8.92	136.81	122.81
1	C	76	VAL	CA-C-N	8.91	136.80	122.81
1	C	76	VAL	C-N-CA	8.91	136.80	122.81
1	B	301	VAL	CA-C-O	-8.87	110.74	120.85
1	C	286	TYR	CA-C-O	-8.87	110.78	120.36
1	A	301	VAL	CA-C-O	-8.87	110.74	120.85
1	B	286	TYR	CA-C-O	-8.85	110.80	120.36
1	D	68	GLY	CA-C-N	8.85	132.50	120.38
1	D	68	GLY	C-N-CA	8.85	132.50	120.38
1	D	286	TYR	CA-C-O	-8.83	110.82	120.36
1	D	301	VAL	CA-C-O	-8.80	110.82	120.85
1	A	68	GLY	CA-C-N	8.79	132.42	120.38
1	A	68	GLY	C-N-CA	8.79	132.42	120.38
1	A	286	TYR	CA-C-O	-8.79	110.87	120.36
1	C	301	VAL	CA-C-O	-8.79	110.83	120.85
1	B	68	GLY	CA-C-N	8.78	132.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	GLY	C-N-CA	8.78	132.41	120.38
1	C	312	ASN	OD1-CG-ND2	8.77	131.37	122.60
1	C	68	GLY	CA-C-N	8.76	132.38	120.38
1	C	68	GLY	C-N-CA	8.76	132.38	120.38
1	A	87	ARG	O-C-N	8.76	134.23	122.59
1	C	171	ARG	CD-NE-CZ	-8.75	112.15	124.40
1	B	87	ARG	O-C-N	8.74	134.21	122.59
1	D	312	ASN	OD1-CG-ND2	8.73	131.33	122.60
1	B	171	ARG	CD-NE-CZ	-8.72	112.19	124.40
1	D	171	ARG	CD-NE-CZ	-8.72	112.19	124.40
1	D	87	ARG	O-C-N	8.71	134.18	122.59
1	A	171	ARG	CD-NE-CZ	-8.70	112.22	124.40
1	A	312	ASN	OD1-CG-ND2	8.70	131.30	122.60
1	C	87	ARG	O-C-N	8.68	134.13	122.59
1	D	260	ARG	CD-NE-CZ	-8.64	112.31	124.40
1	A	260	ARG	CD-NE-CZ	-8.63	112.32	124.40
1	B	260	ARG	CD-NE-CZ	-8.63	112.32	124.40
1	B	312	ASN	OD1-CG-ND2	8.62	131.22	122.60
1	C	260	ARG	CD-NE-CZ	-8.62	112.34	124.40
1	C	29	GLY	O-C-N	-8.61	111.50	122.70
1	A	29	GLY	O-C-N	-8.58	111.54	122.70
1	C	16	LYS	N-CA-C	-8.58	101.74	108.78
1	B	29	GLY	O-C-N	-8.58	111.55	122.70
1	A	316	HIS	CA-C-N	8.57	131.96	120.65
1	A	316	HIS	C-N-CA	8.57	131.96	120.65
1	B	316	HIS	CA-C-N	8.56	131.95	120.65
1	B	316	HIS	C-N-CA	8.56	131.95	120.65
1	D	29	GLY	O-C-N	-8.56	111.57	122.70
1	D	316	HIS	CA-C-N	8.53	131.91	120.65
1	D	316	HIS	C-N-CA	8.53	131.91	120.65
1	D	16	LYS	N-CA-C	-8.51	101.80	108.78
1	D	326	ALA	CB-CA-C	8.50	123.59	109.56
1	B	16	LYS	N-CA-C	-8.50	101.81	108.78
1	B	306	LEU	CA-C-O	8.50	131.31	121.28
1	C	316	HIS	CA-C-N	8.50	131.87	120.65
1	C	316	HIS	C-N-CA	8.50	131.87	120.65
1	C	326	ALA	CB-CA-C	8.50	123.58	109.56
1	A	306	LEU	CA-C-O	8.46	131.27	121.28
1	A	16	LYS	N-CA-C	-8.46	101.84	108.78
1	A	326	ALA	CB-CA-C	8.44	123.49	109.56
1	C	306	LEU	CA-C-O	8.44	131.24	121.28
1	B	326	ALA	CB-CA-C	8.43	123.48	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	LEU	CA-C-O	8.43	131.23	121.28
1	A	296	ASN	CB-CA-C	8.40	122.81	111.14
1	C	296	ASN	CB-CA-C	8.39	122.81	111.14
1	A	206	ILE	CA-C-O	-8.39	111.70	120.51
1	D	296	ASN	CB-CA-C	8.38	122.78	111.14
1	B	206	ILE	CA-C-O	-8.37	111.72	120.51
1	A	22	ARG	CA-C-N	8.37	134.10	123.14
1	A	22	ARG	C-N-CA	8.37	134.10	123.14
1	B	296	ASN	CB-CA-C	8.36	122.76	111.14
1	A	184	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	D	22	ARG	CA-C-N	8.35	134.07	123.14
1	D	22	ARG	C-N-CA	8.35	134.07	123.14
1	B	184	ASN	OD1-CG-ND2	-8.33	114.27	122.60
1	B	22	ARG	CA-C-N	8.32	134.03	123.14
1	B	22	ARG	C-N-CA	8.32	134.03	123.14
1	D	206	ILE	CA-C-O	-8.32	111.78	120.51
1	C	22	ARG	CA-C-N	8.30	134.01	123.14
1	C	22	ARG	C-N-CA	8.30	134.01	123.14
1	D	184	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	D	281	GLY	N-CA-C	-8.27	103.06	114.64
1	A	281	GLY	N-CA-C	-8.26	103.07	114.64
1	C	206	ILE	CA-C-O	-8.26	111.84	120.51
1	C	281	GLY	N-CA-C	-8.25	103.09	114.64
1	C	184	ASN	OD1-CG-ND2	-8.25	114.35	122.60
1	B	281	GLY	N-CA-C	-8.24	103.10	114.64
1	C	112	LYS	N-CA-C	-8.09	103.36	113.55
1	C	141	ASP	N-CA-C	-8.09	102.41	111.71
1	D	141	ASP	N-CA-C	-8.07	102.42	111.71
1	A	108	ASP	CA-C-N	8.06	134.92	122.42
1	A	108	ASP	C-N-CA	8.06	134.92	122.42
1	C	164	ILE	CB-CG1-CD1	-8.06	96.88	113.80
1	B	112	LYS	N-CA-C	-8.05	103.40	113.55
1	B	108	ASP	CA-C-N	8.05	134.90	122.42
1	B	108	ASP	C-N-CA	8.05	134.90	122.42
1	C	108	ASP	CA-C-N	8.05	134.90	122.42
1	C	108	ASP	C-N-CA	8.05	134.90	122.42
1	B	141	ASP	N-CA-C	-8.05	102.46	111.71
1	B	164	ILE	CB-CG1-CD1	-8.05	96.90	113.80
1	D	112	LYS	N-CA-C	-8.04	103.42	113.55
1	D	242	GLU	CA-CB-CG	8.04	130.18	114.10
1	A	141	ASP	N-CA-C	-8.04	102.47	111.71
1	C	84	ASP	N-CA-C	-8.03	102.29	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	GLU	CA-CB-CG	8.03	130.16	114.10
1	A	84	ASP	N-CA-C	-8.02	102.30	113.37
1	A	57	LYS	CA-C-O	-8.02	112.05	120.55
1	C	242	GLU	CA-CB-CG	8.02	130.14	114.10
1	D	57	LYS	CA-C-O	-8.02	112.05	120.55
1	D	108	ASP	CA-C-N	8.02	134.85	122.42
1	D	108	ASP	C-N-CA	8.02	134.85	122.42
1	D	164	ILE	CB-CG1-CD1	-8.02	96.97	113.80
1	A	164	ILE	CB-CG1-CD1	-8.01	96.98	113.80
1	A	112	LYS	N-CA-C	-8.01	103.46	113.55
1	D	84	ASP	N-CA-C	-8.01	102.32	113.37
1	B	57	LYS	CA-C-O	-8.00	112.07	120.55
1	A	161	SER	CA-C-N	7.99	135.88	120.07
1	A	161	SER	C-N-CA	7.99	135.88	120.07
1	B	242	GLU	CA-CB-CG	7.98	130.06	114.10
1	B	161	SER	CA-C-N	7.97	135.85	120.07
1	B	161	SER	C-N-CA	7.97	135.85	120.07
1	C	57	LYS	CA-C-O	-7.97	112.10	120.55
1	C	161	SER	CA-C-N	7.97	135.85	120.07
1	C	161	SER	C-N-CA	7.97	135.85	120.07
1	D	161	SER	CA-C-N	7.97	135.84	120.07
1	D	161	SER	C-N-CA	7.97	135.84	120.07
1	B	84	ASP	N-CA-C	-7.95	102.39	113.37
1	B	165	LEU	N-CA-C	-7.93	103.74	113.50
1	D	165	LEU	N-CA-C	-7.93	103.75	113.50
1	A	76	VAL	CA-C-O	-7.92	111.40	120.67
1	A	270	LEU	CA-C-O	-7.92	112.32	120.71
1	A	165	LEU	N-CA-C	-7.92	103.76	113.50
1	D	270	LEU	CA-C-O	-7.91	112.32	120.71
1	C	165	LEU	N-CA-C	-7.91	103.77	113.50
1	C	76	VAL	CA-C-O	-7.90	111.42	120.67
1	D	76	VAL	CA-C-O	-7.90	111.43	120.67
1	D	309	ASP	N-CA-C	-7.88	103.74	112.72
1	A	309	ASP	N-CA-C	-7.87	103.75	112.72
1	D	32	GLY	CA-C-N	7.85	131.14	120.54
1	D	32	GLY	C-N-CA	7.85	131.14	120.54
1	B	76	VAL	CA-C-O	-7.85	111.49	120.67
1	B	309	ASP	N-CA-C	-7.85	103.78	112.72
1	C	32	GLY	CA-C-N	7.83	131.12	120.54
1	C	32	GLY	C-N-CA	7.83	131.12	120.54
1	A	265	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	B	242	GLU	CA-C-O	-7.82	110.97	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	LEU	CA-C-O	-7.82	112.42	120.71
1	A	32	GLY	CA-C-N	7.82	131.10	120.54
1	A	32	GLY	C-N-CA	7.82	131.10	120.54
1	C	181	ALA	CB-CA-C	7.82	118.69	109.47
1	B	32	GLY	CA-C-N	7.81	131.09	120.54
1	B	32	GLY	C-N-CA	7.81	131.09	120.54
1	B	181	ALA	CB-CA-C	7.81	118.69	109.47
1	B	270	LEU	CA-C-O	-7.81	112.43	120.71
1	C	309	ASP	N-CA-C	-7.80	103.82	112.72
1	C	191	GLY	O-C-N	-7.80	112.56	122.70
1	D	181	ALA	CB-CA-C	7.78	118.64	109.47
1	B	50	LEU	N-CA-CB	-7.77	97.35	110.80
1	B	265	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	A	242	GLU	CA-C-O	-7.76	111.04	119.97
1	A	181	ALA	CB-CA-C	7.75	118.62	109.47
1	D	191	GLY	O-C-N	-7.75	112.62	122.70
1	D	265	ASN	OD1-CG-ND2	-7.75	114.85	122.60
1	C	50	LEU	N-CA-CB	-7.75	97.40	110.80
1	A	284	ASP	CA-C-N	7.74	129.71	121.97
1	A	284	ASP	C-N-CA	7.74	129.71	121.97
1	C	242	GLU	CA-C-O	-7.74	111.07	119.97
1	A	50	LEU	N-CA-CB	-7.73	97.42	110.80
1	A	260	ARG	NE-CZ-NH2	7.72	126.14	119.20
1	D	284	ASP	CA-C-N	7.70	129.67	121.97
1	D	284	ASP	C-N-CA	7.70	129.67	121.97
1	D	50	LEU	N-CA-CB	-7.70	97.48	110.80
1	C	260	ARG	NE-CZ-NH2	7.70	126.13	119.20
1	B	284	ASP	CA-C-N	7.69	129.66	121.97
1	B	284	ASP	C-N-CA	7.69	129.66	121.97
1	D	242	GLU	CA-C-O	-7.69	111.12	119.97
1	B	260	ARG	NE-CZ-NH2	7.68	126.12	119.20
1	C	284	ASP	CA-C-N	7.68	129.65	121.97
1	C	284	ASP	C-N-CA	7.68	129.65	121.97
1	A	191	GLY	O-C-N	-7.67	112.72	122.70
1	B	191	GLY	O-C-N	-7.67	112.73	122.70
1	D	260	ARG	NE-CZ-NH2	7.67	126.10	119.20
1	C	265	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	C	156	GLU	N-CA-C	-7.64	103.06	113.30
1	C	134	LEU	CB-CA-C	7.63	123.02	110.74
1	B	134	LEU	CB-CA-C	7.62	123.02	110.74
1	A	78	ILE	CA-CB-CG1	7.61	123.33	110.40
1	A	134	LEU	CB-CA-C	7.61	122.99	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	GLU	N-CA-C	-7.60	103.11	113.30
1	D	134	LEU	CB-CA-C	7.58	122.95	110.74
1	C	70	VAL	CA-C-N	7.58	135.00	121.66
1	C	70	VAL	C-N-CA	7.58	135.00	121.66
1	A	294	ASN	CA-C-O	-7.57	113.18	121.28
1	D	70	VAL	CA-C-N	7.57	134.97	121.66
1	D	70	VAL	C-N-CA	7.57	134.97	121.66
1	A	70	VAL	CA-C-N	7.56	134.97	121.66
1	A	70	VAL	C-N-CA	7.56	134.97	121.66
1	D	78	ILE	CA-CB-CG1	7.56	123.26	110.40
1	B	70	VAL	CA-C-N	7.56	134.96	121.66
1	B	70	VAL	C-N-CA	7.56	134.96	121.66
1	A	156	GLU	N-CA-C	-7.55	103.18	113.30
1	B	78	ILE	CA-CB-CG1	7.55	123.23	110.40
1	C	78	ILE	CA-CB-CG1	7.54	123.22	110.40
1	D	294	ASN	CA-C-O	-7.54	113.21	121.28
1	B	52	ASP	CA-C-O	-7.54	112.55	120.99
1	B	124	VAL	N-CA-C	-7.53	102.03	112.50
1	C	327	ARG	CD-NE-CZ	-7.53	113.86	124.40
1	B	156	GLU	N-CA-C	-7.53	103.22	113.30
1	D	327	ARG	CD-NE-CZ	-7.52	113.87	124.40
1	B	294	ASN	CA-C-O	-7.51	113.24	121.28
1	D	124	VAL	N-CA-C	-7.51	102.06	112.50
1	D	251	ILE	CA-C-O	-7.51	113.60	121.41
1	C	124	VAL	N-CA-C	-7.51	102.06	112.50
1	A	327	ARG	CD-NE-CZ	-7.50	113.89	124.40
1	A	52	ASP	CA-C-O	-7.49	112.60	120.99
1	B	251	ILE	CA-C-O	-7.49	113.62	121.41
1	A	124	VAL	N-CA-C	-7.49	102.09	112.50
1	B	195	ASP	CA-CB-CG	-7.48	105.12	112.60
1	C	251	ILE	CA-C-O	-7.47	113.64	121.41
1	D	266	GLU	CB-CG-CD	7.47	125.30	112.60
1	D	52	ASP	CA-C-O	-7.46	112.63	120.99
1	B	327	ARG	CD-NE-CZ	-7.46	113.96	124.40
1	D	287	ILE	N-CA-CB	-7.46	101.24	112.35
1	B	266	GLU	CB-CG-CD	7.45	125.27	112.60
1	C	266	GLU	CB-CG-CD	7.45	125.27	112.60
1	C	52	ASP	CA-C-O	-7.44	112.66	120.99
1	D	326	ALA	N-CA-C	-7.43	103.83	113.12
1	A	195	ASP	CA-CB-CG	-7.43	105.17	112.60
1	A	266	GLU	CB-CG-CD	7.43	125.23	112.60
1	C	294	ASN	CA-C-O	-7.42	113.34	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ILE	N-CA-CB	-7.41	101.31	112.35
1	C	195	ASP	CA-CB-CG	-7.41	105.19	112.60
1	B	287	ILE	N-CA-CB	-7.41	101.31	112.35
1	C	287	ILE	N-CA-CB	-7.41	101.32	112.35
1	A	251	ILE	CA-C-O	-7.40	113.71	121.41
1	B	77	ASP	CA-C-O	-7.40	112.75	121.11
1	C	326	ALA	N-CA-C	-7.39	103.88	113.12
1	B	236	ALA	CA-C-N	7.39	130.40	120.65
1	B	236	ALA	C-N-CA	7.39	130.40	120.65
1	C	236	ALA	CA-C-N	7.38	130.40	120.65
1	C	236	ALA	C-N-CA	7.38	130.40	120.65
1	A	326	ALA	N-CA-C	-7.38	103.89	113.12
1	A	236	ALA	CA-C-N	7.38	130.38	120.65
1	A	236	ALA	C-N-CA	7.38	130.38	120.65
1	C	89	ALA	N-CA-CB	-7.37	98.15	109.94
1	D	195	ASP	CA-CB-CG	-7.35	105.25	112.60
1	B	89	ALA	N-CA-CB	-7.35	98.18	109.94
1	D	236	ALA	CA-C-N	7.35	130.35	120.65
1	D	236	ALA	C-N-CA	7.35	130.35	120.65
1	A	77	ASP	CA-C-O	-7.34	112.82	121.11
1	B	326	ALA	N-CA-C	-7.33	103.96	113.12
1	D	89	ALA	N-CA-CB	-7.31	98.24	109.94
1	A	89	ALA	N-CA-CB	-7.30	98.26	109.94
1	C	323	SER	N-CA-CB	-7.30	100.88	110.59
1	A	163	THR	CA-CB-OG1	-7.29	98.67	109.60
1	D	77	ASP	CA-C-O	-7.27	112.89	121.11
1	D	323	SER	N-CA-CB	-7.26	100.94	110.59
1	B	323	SER	N-CA-CB	-7.25	100.95	110.59
1	C	77	ASP	CA-C-O	-7.24	112.92	121.11
1	C	309	ASP	OD1-CG-OD2	-7.24	105.53	122.90
1	A	309	ASP	OD1-CG-OD2	-7.23	105.54	122.90
1	A	323	SER	N-CA-CB	-7.23	100.97	110.59
1	D	309	ASP	OD1-CG-OD2	-7.23	105.55	122.90
1	C	280	TYR	N-CA-C	-7.23	104.35	113.02
1	B	309	ASP	OD1-CG-OD2	-7.22	105.58	122.90
1	C	163	THR	CA-CB-OG1	-7.20	98.79	109.60
1	B	163	THR	CA-CB-OG1	-7.20	98.80	109.60
1	C	202	SER	CA-C-O	-7.19	111.70	119.97
1	D	280	TYR	N-CA-C	-7.19	104.39	113.02
1	B	280	TYR	N-CA-C	-7.18	104.40	113.02
1	B	202	SER	CA-C-O	-7.18	111.71	119.97
1	D	202	SER	CA-C-O	-7.18	111.71	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	THR	CA-CB-OG1	-7.18	98.83	109.60
1	A	202	SER	CA-C-O	-7.17	111.72	119.97
1	A	280	TYR	N-CA-C	-7.17	104.42	113.02
1	D	56	SER	CA-C-N	7.16	129.88	120.28
1	D	56	SER	C-N-CA	7.16	129.88	120.28
1	D	113	ASN	CA-CB-CG	-7.16	105.44	112.60
1	C	113	ASN	CA-CB-CG	-7.15	105.45	112.60
1	C	56	SER	CA-C-N	7.14	129.85	120.28
1	C	56	SER	C-N-CA	7.14	129.85	120.28
1	D	186	HIS	CA-CB-CG	-7.14	106.66	113.80
1	C	186	HIS	CA-CB-CG	-7.12	106.68	113.80
1	B	22	ARG	CD-NE-CZ	-7.12	114.44	124.40
1	C	22	ARG	CD-NE-CZ	-7.12	114.44	124.40
1	C	144	THR	N-CA-CB	7.12	121.26	110.30
1	A	186	HIS	CA-CB-CG	-7.11	106.69	113.80
1	B	113	ASN	CA-CB-CG	-7.11	105.49	112.60
1	A	113	ASN	CA-CB-CG	-7.11	105.49	112.60
1	D	22	ARG	CD-NE-CZ	-7.11	114.45	124.40
1	C	110	VAL	CA-C-O	-7.11	113.66	121.05
1	A	56	SER	CA-C-N	7.09	129.79	120.28
1	A	56	SER	C-N-CA	7.09	129.79	120.28
1	D	144	THR	N-CA-CB	7.09	121.22	110.30
1	D	242	GLU	CB-CG-CD	7.09	124.65	112.60
1	B	56	SER	CA-C-N	7.09	129.78	120.28
1	B	56	SER	C-N-CA	7.09	129.78	120.28
1	B	110	VAL	CA-C-O	-7.09	113.68	121.05
1	A	144	THR	N-CA-CB	7.08	121.21	110.30
1	B	144	THR	N-CA-CB	7.07	121.19	110.30
1	B	186	HIS	CA-CB-CG	-7.07	106.73	113.80
1	A	22	ARG	CD-NE-CZ	-7.07	114.51	124.40
1	A	59	ILE	N-CA-C	-7.07	103.64	110.42
1	C	242	GLU	CB-CG-CD	7.06	124.60	112.60
1	C	129	PHE	CA-C-N	7.06	133.69	122.11
1	C	129	PHE	C-N-CA	7.06	133.69	122.11
1	A	242	GLU	CB-CG-CD	7.05	124.58	112.60
1	D	129	PHE	CA-C-N	7.05	133.67	122.11
1	D	129	PHE	C-N-CA	7.05	133.67	122.11
1	B	129	PHE	CA-C-N	7.04	133.66	122.11
1	B	129	PHE	C-N-CA	7.04	133.66	122.11
1	A	110	VAL	CA-C-O	-7.04	113.73	121.05
1	D	110	VAL	CA-C-O	-7.03	113.74	121.05
1	A	129	PHE	CA-C-N	7.03	133.64	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	PHE	C-N-CA	7.03	133.64	122.11
1	B	242	GLU	CB-CG-CD	7.02	124.53	112.60
1	C	59	ILE	N-CA-C	-7.00	103.70	110.42
1	D	59	ILE	N-CA-C	-6.99	103.71	110.42
1	C	44	ILE	CA-C-O	-6.98	112.31	120.83
1	B	111	ASP	CB-CG-OD1	6.95	134.39	118.40
1	A	111	ASP	CB-CG-OD1	6.95	134.38	118.40
1	D	44	ILE	CA-C-O	-6.95	112.35	120.83
1	C	111	ASP	CB-CG-OD1	6.94	134.36	118.40
1	B	44	ILE	CA-C-O	-6.93	112.37	120.83
1	D	111	ASP	CB-CG-OD1	6.93	134.33	118.40
1	C	258	VAL	CB-CA-C	-6.92	102.97	112.04
1	B	59	ILE	N-CA-C	-6.92	103.78	110.42
1	B	284	ASP	O-C-N	6.90	131.77	122.59
1	C	256	ALA	CA-C-N	6.89	130.01	120.63
1	C	256	ALA	C-N-CA	6.89	130.01	120.63
1	B	256	ALA	CA-C-N	6.89	130.00	120.63
1	B	256	ALA	C-N-CA	6.89	130.00	120.63
1	D	114	ILE	CB-CG1-CD1	6.89	128.27	113.80
1	C	114	ILE	CB-CG1-CD1	6.89	128.27	113.80
1	B	114	ILE	CB-CG1-CD1	6.89	128.26	113.80
1	B	258	VAL	CB-CA-C	-6.88	103.02	112.04
1	A	114	ILE	CB-CG1-CD1	6.88	128.24	113.80
1	D	256	ALA	CA-C-N	6.87	129.97	120.63
1	D	256	ALA	C-N-CA	6.87	129.97	120.63
1	D	258	VAL	CB-CA-C	-6.87	103.04	112.04
1	C	284	ASP	O-C-N	6.86	131.72	122.59
1	A	44	ILE	CA-C-O	-6.85	112.47	120.83
1	B	38	ALA	CA-C-O	6.85	127.88	120.55
1	A	258	VAL	CB-CA-C	-6.84	103.08	112.04
1	A	256	ALA	CA-C-N	6.83	129.93	120.63
1	A	256	ALA	C-N-CA	6.83	129.93	120.63
1	D	284	ASP	O-C-N	6.83	131.67	122.59
1	A	38	ALA	CA-C-O	6.83	127.85	120.55
1	B	312	ASN	CA-CB-CG	-6.82	105.78	112.60
1	A	284	ASP	O-C-N	6.81	131.65	122.59
1	C	260	ARG	CA-C-O	-6.81	113.61	120.90
1	C	38	ALA	CA-C-O	6.81	127.83	120.55
1	A	159	ILE	CA-C-O	-6.80	113.96	121.92
1	C	159	ILE	O-C-N	6.80	129.83	122.76
1	C	312	ASN	CA-CB-CG	-6.79	105.81	112.60
1	B	260	ARG	CA-C-O	-6.79	113.64	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	ARG	CA-C-O	-6.79	113.64	120.90
1	D	38	ALA	CA-C-O	6.79	127.81	120.55
1	C	159	ILE	CA-C-O	-6.78	113.99	121.92
1	D	312	ASN	CA-CB-CG	-6.77	105.83	112.60
1	B	159	ILE	CA-C-O	-6.76	114.01	121.92
1	A	260	ARG	CA-C-O	-6.76	113.66	120.90
1	D	249	TYR	CB-CG-CD1	6.75	130.93	120.80
1	A	159	ILE	O-C-N	6.74	129.77	122.76
1	A	312	ASN	CA-CB-CG	-6.73	105.87	112.60
1	C	249	TYR	CB-CG-CD1	6.72	130.88	120.80
1	D	159	ILE	O-C-N	6.72	129.75	122.76
1	B	184	ASN	CA-CB-CG	6.72	119.32	112.60
1	B	159	ILE	O-C-N	6.71	129.74	122.76
1	D	184	ASN	CA-CB-CG	6.71	119.31	112.60
1	D	74	LYS	CB-CA-C	-6.70	96.97	110.17
1	D	159	ILE	CA-C-O	-6.70	114.08	121.92
1	A	74	LYS	CB-CA-C	-6.70	96.97	110.17
1	B	249	TYR	CB-CG-CD1	6.70	130.85	120.80
1	B	232	ASN	CA-CB-CG	-6.69	105.91	112.60
1	A	249	TYR	CB-CG-CD1	6.68	130.82	120.80
1	C	184	ASN	CA-CB-CG	6.68	119.28	112.60
1	C	74	LYS	CB-CA-C	-6.68	97.01	110.17
1	D	227	GLU	CA-C-N	6.66	131.67	120.88
1	D	227	GLU	C-N-CA	6.66	131.67	120.88
1	C	232	ASN	CA-CB-CG	-6.66	105.94	112.60
1	B	74	LYS	CB-CA-C	-6.64	97.09	110.17
1	A	184	ASN	CA-CB-CG	6.64	119.24	112.60
1	A	227	GLU	CA-C-N	6.62	131.61	120.88
1	A	227	GLU	C-N-CA	6.62	131.61	120.88
1	B	227	GLU	CA-C-N	6.62	131.60	120.88
1	B	227	GLU	C-N-CA	6.62	131.60	120.88
1	A	232	ASN	CA-CB-CG	-6.62	105.98	112.60
1	D	232	ASN	CA-CB-CG	-6.61	105.99	112.60
1	A	58	ALA	CA-C-N	6.60	128.88	120.56
1	A	58	ALA	C-N-CA	6.60	128.88	120.56
1	C	227	GLU	CA-C-N	6.60	131.57	120.88
1	C	227	GLU	C-N-CA	6.60	131.57	120.88
1	A	163	THR	CA-CB-CG2	6.59	121.70	110.50
1	C	58	ALA	CA-C-N	6.58	128.86	120.56
1	C	58	ALA	C-N-CA	6.58	128.86	120.56
1	C	133	PHE	CA-C-N	-6.57	113.48	123.07
1	C	133	PHE	C-N-CA	-6.57	113.48	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ALA	CA-C-N	6.56	128.83	120.56
1	D	58	ALA	C-N-CA	6.56	128.83	120.56
1	B	50	LEU	CB-CA-C	6.56	121.57	109.70
1	B	163	THR	CA-CB-CG2	6.56	121.64	110.50
1	A	50	LEU	CB-CA-C	6.55	121.56	109.70
1	D	163	THR	CA-CB-CG2	6.55	121.63	110.50
1	C	163	THR	CA-CB-CG2	6.54	121.62	110.50
1	C	267	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	D	50	LEU	CB-CA-C	6.54	121.53	109.70
1	D	133	PHE	CA-C-N	-6.54	113.52	123.07
1	D	133	PHE	C-N-CA	-6.54	113.52	123.07
1	B	58	ALA	CA-C-N	6.53	128.79	120.56
1	B	58	ALA	C-N-CA	6.53	128.79	120.56
1	C	50	LEU	CB-CA-C	6.53	121.52	109.70
1	D	267	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	133	PHE	CA-C-N	-6.51	113.57	123.07
1	A	133	PHE	C-N-CA	-6.51	113.57	123.07
1	B	133	PHE	CA-C-N	-6.51	113.56	123.07
1	B	133	PHE	C-N-CA	-6.51	113.56	123.07
1	C	61	ASP	CA-C-N	-6.50	110.92	120.28
1	C	61	ASP	C-N-CA	-6.50	110.92	120.28
1	B	61	ASP	CA-C-N	-6.49	110.93	120.28
1	B	61	ASP	C-N-CA	-6.49	110.93	120.28
1	B	243	LYS	N-CA-CB	6.47	120.39	110.61
1	C	243	LYS	N-CA-CB	6.47	120.39	110.61
1	A	243	LYS	N-CA-CB	6.47	120.38	110.61
1	A	267	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	D	61	ASP	CA-C-N	-6.46	110.98	120.28
1	D	61	ASP	C-N-CA	-6.46	110.98	120.28
1	A	61	ASP	CA-C-N	-6.45	110.99	120.28
1	A	61	ASP	C-N-CA	-6.45	110.99	120.28
1	A	226	LEU	N-CA-C	-6.45	105.57	113.50
1	D	243	LYS	N-CA-CB	6.45	120.34	110.61
1	C	228	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	B	228	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	D	228	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	B	267	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	B	226	LEU	N-CA-C	-6.40	105.63	113.50
1	A	78	ILE	N-CA-C	-6.39	99.92	108.35
1	A	228	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	B	58	ALA	CA-C-O	6.37	127.30	119.97
1	A	58	ALA	CA-C-O	6.36	127.29	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	LEU	CA-C-O	-6.36	113.83	120.70
1	D	226	LEU	N-CA-C	-6.36	105.67	113.50
1	D	78	ILE	N-CA-C	-6.36	99.96	108.35
1	B	271	THR	CA-C-O	-6.33	114.75	122.41
1	C	226	LEU	N-CA-C	-6.33	105.71	113.50
1	A	132	LEU	CA-C-O	-6.33	113.86	120.70
1	B	78	ILE	N-CA-C	-6.33	99.99	108.35
1	C	279	LEU	CA-C-N	-6.33	111.67	122.56
1	C	279	LEU	C-N-CA	-6.33	111.67	122.56
1	C	78	ILE	N-CA-C	-6.33	100.00	108.35
1	A	271	THR	CA-C-O	-6.32	114.76	122.41
1	C	58	ALA	CA-C-O	6.32	127.23	119.97
1	D	58	ALA	CA-C-O	6.30	127.22	119.97
1	A	265	ASN	CA-C-O	-6.30	114.53	121.84
1	D	279	LEU	CA-C-N	-6.29	111.75	122.56
1	D	279	LEU	C-N-CA	-6.29	111.75	122.56
1	C	271	THR	CA-C-O	-6.29	114.80	122.41
1	A	30	PHE	O-C-N	-6.28	115.60	122.07
1	A	235	ASP	CA-C-O	-6.28	110.36	120.65
1	B	265	ASN	CA-C-O	-6.27	114.56	121.84
1	B	279	LEU	CA-C-N	-6.27	111.77	122.56
1	B	279	LEU	C-N-CA	-6.27	111.77	122.56
1	D	271	THR	CA-C-O	-6.27	114.83	122.41
1	C	132	LEU	CA-C-O	-6.26	113.94	120.70
1	A	294	ASN	CA-C-N	6.26	129.52	120.38
1	A	294	ASN	C-N-CA	6.26	129.52	120.38
1	D	305	GLU	CG-CD-OE2	-6.26	104.01	118.40
1	A	305	GLU	CG-CD-OE2	-6.25	104.02	118.40
1	A	279	LEU	CA-C-N	-6.25	111.81	122.56
1	A	279	LEU	C-N-CA	-6.25	111.81	122.56
1	C	305	GLU	CG-CD-OE2	-6.25	104.02	118.40
1	C	30	PHE	O-C-N	-6.25	115.63	122.07
1	A	127	SER	N-CA-C	-6.24	105.94	112.93
1	D	265	ASN	CA-C-O	-6.24	114.60	121.84
1	D	283	ARG	CA-C-O	-6.24	111.81	119.18
1	B	87	ARG	CA-C-O	-6.24	111.59	120.51
1	D	30	PHE	O-C-N	-6.24	115.64	122.07
1	D	230	PHE	N-CA-CB	6.24	119.39	110.16
1	B	230	PHE	N-CA-CB	6.23	119.38	110.16
1	B	305	GLU	CG-CD-OE2	-6.23	104.07	118.40
1	D	294	ASN	CA-C-N	6.23	129.47	120.38
1	D	294	ASN	C-N-CA	6.23	129.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PHE	N-CA-CB	6.23	119.38	110.16
1	D	132	LEU	CA-C-O	-6.23	113.97	120.70
1	B	294	ASN	CA-C-N	6.22	129.47	120.38
1	B	294	ASN	C-N-CA	6.22	129.47	120.38
1	A	87	ARG	CA-C-O	-6.22	111.61	120.51
1	A	283	ARG	CA-C-O	-6.22	111.84	119.18
1	D	127	SER	N-CA-C	-6.22	105.97	112.93
1	A	313	ARG	CG-CD-NE	6.22	125.67	112.00
1	C	127	SER	N-CA-C	-6.22	105.97	112.93
1	B	235	ASP	CA-C-O	-6.21	110.46	120.65
1	C	235	ASP	CA-C-O	-6.21	110.46	120.65
1	C	283	ARG	CA-C-O	-6.21	111.85	119.18
1	D	313	ARG	CG-CD-NE	6.21	125.66	112.00
1	C	294	ASN	CA-C-N	6.21	129.44	120.38
1	C	294	ASN	C-N-CA	6.21	129.44	120.38
1	D	235	ASP	CA-C-O	-6.20	110.49	120.65
1	B	30	PHE	O-C-N	-6.19	115.69	122.07
1	C	265	ASN	CA-C-O	-6.19	114.66	121.84
1	B	127	SER	N-CA-C	-6.18	106.00	112.93
1	C	313	ARG	CG-CD-NE	6.18	125.60	112.00
1	B	313	ARG	CG-CD-NE	6.18	125.60	112.00
1	B	283	ARG	CA-C-O	-6.17	111.89	119.18
1	C	87	ARG	CA-C-O	-6.17	111.69	120.51
1	A	132	LEU	N-CA-CB	-6.16	100.11	110.83
1	C	230	PHE	N-CA-CB	6.15	119.27	110.16
1	D	87	ARG	CA-C-O	-6.15	111.71	120.51
1	B	284	ASP	CA-C-O	-6.15	111.72	120.51
1	B	132	LEU	N-CA-CB	-6.14	100.14	110.83
1	D	109	LEU	O-C-N	6.14	129.44	122.19
1	C	292	VAL	CA-CB-CG2	6.14	120.84	110.40
1	D	292	VAL	CA-CB-CG2	6.14	120.84	110.40
1	B	311	LYS	O-C-N	6.14	130.75	122.59
1	C	109	LEU	O-C-N	6.14	129.43	122.19
1	A	109	LEU	O-C-N	6.14	129.43	122.19
1	D	132	LEU	N-CA-CB	-6.13	100.16	110.83
1	D	63	MET	N-CA-CB	6.13	119.21	110.13
1	B	109	LEU	O-C-N	6.12	129.42	122.19
1	D	309	ASP	CA-C-N	6.12	133.23	121.54
1	D	309	ASP	C-N-CA	6.12	133.23	121.54
1	A	311	LYS	O-C-N	6.11	130.72	122.59
1	B	292	VAL	CA-CB-CG2	6.11	120.78	110.40
1	A	309	ASP	CA-C-N	6.11	133.21	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ASP	C-N-CA	6.11	133.21	121.54
1	C	63	MET	N-CA-CB	6.10	119.16	110.13
1	C	294	ASN	CB-CA-C	6.10	121.93	110.95
1	B	309	ASP	CA-C-N	6.10	133.19	121.54
1	B	309	ASP	C-N-CA	6.10	133.19	121.54
1	C	132	LEU	N-CA-CB	-6.09	100.22	110.83
1	D	311	LYS	O-C-N	6.09	130.70	122.59
1	C	284	ASP	CA-C-O	-6.09	111.80	120.51
1	A	292	VAL	CA-CB-CG2	6.09	120.75	110.40
1	C	311	LYS	O-C-N	6.09	130.69	122.59
1	B	63	MET	N-CA-CB	6.08	119.14	110.13
1	A	63	MET	N-CA-CB	6.08	119.13	110.13
1	A	269	ILE	N-CA-CB	6.08	118.59	111.66
1	D	284	ASP	CA-C-O	-6.08	111.81	120.51
1	A	284	ASP	CA-C-O	-6.08	111.82	120.51
1	D	197	GLU	CB-CG-CD	6.08	122.94	112.60
1	A	226	LEU	CA-C-O	-6.07	112.46	119.14
1	B	197	GLU	CB-CG-CD	6.07	122.92	112.60
1	A	197	GLU	CB-CG-CD	6.07	122.92	112.60
1	C	309	ASP	CA-C-N	6.07	133.13	121.54
1	C	309	ASP	C-N-CA	6.07	133.13	121.54
1	D	116	ILE	N-CA-C	-6.07	104.83	110.53
1	B	269	ILE	N-CA-CB	6.07	118.57	111.66
1	C	116	ILE	N-CA-C	-6.07	104.83	110.53
1	D	109	LEU	CB-CA-C	-6.07	100.14	110.88
1	B	294	ASN	CB-CA-C	6.06	121.85	110.95
1	B	150	PHE	CA-C-O	-6.06	111.80	119.31
1	C	109	LEU	CB-CA-C	-6.05	100.17	110.88
1	C	197	GLU	CB-CG-CD	6.05	122.89	112.60
1	A	109	LEU	CB-CA-C	-6.04	100.18	110.88
1	C	150	PHE	CA-C-O	-6.04	111.82	119.31
1	B	226	LEU	CA-C-O	-6.04	112.49	119.14
1	A	294	ASN	CB-CA-C	6.04	121.82	110.95
1	A	157	ARG	CG-CD-NE	6.03	125.27	112.00
1	C	269	ILE	N-CA-CB	6.03	118.53	111.66
1	B	109	LEU	CB-CA-C	-6.02	100.22	110.88
1	A	139	PRO	CA-C-N	6.02	128.15	120.56
1	A	139	PRO	C-N-CA	6.02	128.15	120.56
1	B	184	ASN	N-CA-C	-6.02	106.07	113.41
1	D	269	ILE	N-CA-CB	6.02	118.52	111.66
1	A	293	ILE	CA-C-O	-6.01	113.77	121.40
1	B	157	ARG	CG-CD-NE	6.01	125.21	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	226	LEU	CA-C-O	-6.01	112.53	119.14
1	D	294	ASN	CB-CA-C	6.01	121.76	110.95
1	D	302	ILE	CB-CG1-CD1	-6.01	101.19	113.80
1	D	150	PHE	CA-C-O	-6.00	111.87	119.31
1	C	184	ASN	N-CA-C	-6.00	106.09	113.41
1	D	293	ILE	CA-C-O	-5.99	113.79	121.40
1	A	150	PHE	CA-C-O	-5.99	111.88	119.31
1	C	86	CYS	N-CA-CB	-5.99	102.90	110.45
1	A	235	ASP	N-CA-C	-5.99	104.11	112.25
1	C	293	ILE	CA-C-O	-5.99	113.80	121.40
1	A	302	ILE	CB-CG1-CD1	-5.98	101.24	113.80
1	B	235	ASP	N-CA-C	-5.98	104.12	112.25
1	D	184	ASN	N-CA-C	-5.98	106.11	113.41
1	B	116	ILE	N-CA-C	-5.98	104.91	110.53
1	D	139	PRO	CA-C-N	5.98	128.09	120.56
1	D	139	PRO	C-N-CA	5.98	128.09	120.56
1	A	40	MET	O-C-N	5.97	128.30	122.09
1	A	184	ASN	N-CA-C	-5.97	106.13	113.41
1	C	157	ARG	CG-CD-NE	5.97	125.13	112.00
1	C	302	ILE	CB-CG1-CD1	-5.96	101.28	113.80
1	D	86	CYS	N-CA-CB	-5.96	102.94	110.45
1	D	272	VAL	CA-C-N	5.96	131.59	122.77
1	D	272	VAL	C-N-CA	5.96	131.59	122.77
1	B	272	VAL	CA-C-N	5.95	131.58	122.77
1	B	272	VAL	C-N-CA	5.95	131.58	122.77
1	D	157	ARG	CG-CD-NE	5.95	125.09	112.00
1	A	116	ILE	N-CA-C	-5.95	104.94	110.53
1	B	86	CYS	N-CA-CB	-5.95	102.95	110.45
1	B	293	ILE	CA-C-O	-5.95	113.85	121.40
1	C	226	LEU	CA-C-O	-5.95	112.60	119.14
1	C	272	VAL	CA-C-N	5.95	131.57	122.77
1	C	272	VAL	C-N-CA	5.95	131.57	122.77
1	B	302	ILE	CB-CG1-CD1	-5.94	101.32	113.80
1	A	237	ALA	O-C-N	5.94	128.21	122.03
1	C	235	ASP	N-CA-C	-5.94	104.18	112.25
1	C	139	PRO	CA-C-N	5.93	128.04	120.56
1	C	139	PRO	C-N-CA	5.93	128.04	120.56
1	B	111	ASP	O-C-N	5.93	129.65	122.35
1	D	40	MET	O-C-N	5.93	128.26	122.09
1	B	116	ILE	O-C-N	5.93	128.06	121.90
1	B	64	ASP	CA-CB-CG	-5.92	106.68	112.60
1	B	40	MET	O-C-N	5.92	128.25	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	VAL	CA-C-N	5.91	131.52	122.77
1	A	272	VAL	C-N-CA	5.91	131.52	122.77
1	A	86	CYS	N-CA-CB	-5.91	103.00	110.45
1	B	237	ALA	O-C-N	5.91	128.17	122.03
1	C	64	ASP	CA-CB-CG	-5.91	106.69	112.60
1	C	263	LEU	CA-C-O	-5.89	113.19	119.97
1	C	116	ILE	O-C-N	5.89	128.03	121.90
1	C	119	SER	CA-CB-OG	-5.89	99.32	111.10
1	D	119	SER	CA-CB-OG	-5.89	99.31	111.10
1	A	116	ILE	O-C-N	5.89	128.02	121.90
1	C	111	ASP	O-C-N	5.89	129.59	122.35
1	D	235	ASP	N-CA-C	-5.89	104.25	112.25
1	A	111	ASP	O-C-N	5.88	129.59	122.35
1	D	122	GLU	O-C-N	5.88	128.12	122.07
1	D	299	ARG	NH1-CZ-NH2	5.88	126.94	119.30
1	B	119	SER	CA-CB-OG	-5.87	99.35	111.10
1	C	237	ALA	O-C-N	5.87	128.13	122.03
1	D	324	VAL	N-CA-C	-5.87	103.75	111.09
1	A	119	SER	CA-CB-OG	-5.87	99.36	111.10
1	D	237	ALA	O-C-N	5.87	128.13	122.03
1	A	299	ARG	NH1-CZ-NH2	5.87	126.93	119.30
1	B	307	ASN	N-CA-CB	-5.86	100.58	110.49
1	D	116	ILE	O-C-N	5.86	128.00	121.90
1	C	211	ILE	N-CA-CB	-5.86	101.54	111.50
1	B	139	PRO	CA-C-N	5.86	128.15	120.60
1	B	139	PRO	C-N-CA	5.86	128.15	120.60
1	C	40	MET	O-C-N	5.86	128.18	122.09
1	D	62	ALA	CA-C-O	-5.86	113.48	120.10
1	A	64	ASP	CA-CB-CG	-5.85	106.75	112.60
1	A	67	HIS	CA-C-O	-5.85	113.24	119.97
1	D	309	ASP	N-CA-CB	5.85	119.42	110.70
1	A	309	ASP	N-CA-CB	5.85	119.41	110.70
1	A	263	LEU	CA-C-O	-5.84	113.25	119.97
1	D	67	HIS	CA-C-O	-5.84	113.25	119.97
1	B	211	ILE	N-CA-CB	-5.84	101.57	111.50
1	B	299	ARG	NH1-CZ-NH2	5.84	126.89	119.30
1	D	111	ASP	O-C-N	5.84	129.53	122.35
1	A	211	ILE	N-CA-CB	-5.84	101.58	111.50
1	A	176	GLU	CA-C-O	5.83	126.43	119.60
1	D	307	ASN	N-CA-CB	-5.83	100.63	110.49
1	C	89	ALA	CA-C-O	-5.83	114.01	120.60
1	A	280	TYR	CA-C-N	-5.83	113.42	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	TYR	C-N-CA	-5.83	113.42	122.69
1	C	260	ARG	N-CA-CB	5.83	118.62	109.94
1	D	211	ILE	N-CA-CB	-5.83	101.59	111.50
1	C	307	ASN	N-CA-CB	-5.83	100.64	110.49
1	D	64	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	123	SER	N-CA-C	5.82	119.64	112.54
1	B	260	ARG	N-CA-CB	5.82	118.61	109.94
1	C	299	ARG	NH1-CZ-NH2	5.82	126.87	119.30
1	A	324	VAL	N-CA-C	-5.82	103.82	111.09
1	D	263	LEU	CA-C-O	-5.82	113.28	119.97
1	A	89	ALA	CA-C-O	-5.82	114.03	120.60
1	B	123	SER	N-CA-C	5.82	119.63	112.54
1	C	62	ALA	CA-C-O	-5.81	113.53	120.10
1	C	67	HIS	CA-C-O	-5.81	113.29	119.97
1	D	166	ASP	O-C-N	5.81	128.06	122.07
1	A	307	ASN	N-CA-CB	-5.81	100.67	110.49
1	B	263	LEU	CA-C-O	-5.80	113.29	119.97
1	C	176	GLU	CA-C-O	5.80	126.39	119.60
1	D	176	GLU	CA-C-O	5.80	126.39	119.60
1	B	89	ALA	CA-C-O	-5.80	114.05	120.60
1	C	285	VAL	CB-CA-C	-5.80	106.29	111.74
1	D	280	TYR	CA-C-N	-5.80	113.47	122.69
1	D	280	TYR	C-N-CA	-5.80	113.47	122.69
1	C	309	ASP	N-CA-CB	5.79	119.33	110.70
1	D	123	SER	N-CA-C	5.79	119.61	112.54
1	C	324	VAL	N-CA-C	-5.79	103.85	111.09
1	A	122	GLU	O-C-N	5.79	128.03	122.07
1	A	138	ASN	CB-CG-ND2	5.78	125.07	116.40
1	B	176	GLU	CA-C-O	5.78	126.36	119.60
1	B	324	VAL	N-CA-C	-5.78	103.86	111.09
1	B	280	TYR	CA-C-N	-5.78	113.50	122.69
1	B	280	TYR	C-N-CA	-5.78	113.50	122.69
1	C	122	GLU	O-C-N	5.78	128.02	122.07
1	A	63	MET	O-C-N	5.77	129.16	122.17
1	B	67	HIS	CA-C-O	-5.77	113.33	119.97
1	C	280	TYR	CA-C-N	-5.77	113.51	122.69
1	C	280	TYR	C-N-CA	-5.77	113.51	122.69
1	B	138	ASN	CB-CG-ND2	5.77	125.06	116.40
1	A	62	ALA	CA-C-O	-5.77	113.58	120.10
1	A	166	ASP	O-C-N	5.77	128.01	122.07
1	B	309	ASP	N-CA-CB	5.77	119.29	110.70
1	B	50	LEU	CA-C-N	5.77	131.00	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	LEU	C-N-CA	5.77	131.00	122.99
1	D	313	ARG	CB-CA-C	5.76	121.10	110.56
1	D	89	ALA	CA-C-O	-5.76	114.09	120.60
1	C	138	ASN	CB-CG-ND2	5.76	125.03	116.40
1	A	50	LEU	CA-C-N	5.75	130.98	122.99
1	A	50	LEU	C-N-CA	5.75	130.98	122.99
1	D	198	LEU	O-C-N	5.75	126.03	121.55
1	C	123	SER	N-CA-C	5.75	119.55	112.54
1	C	198	LEU	O-C-N	5.75	126.03	121.55
1	C	313	ARG	CB-CA-C	5.75	121.07	110.56
1	B	63	MET	O-C-N	5.74	129.12	122.17
1	D	285	VAL	CB-CA-C	-5.74	106.34	111.74
1	A	260	ARG	N-CA-CB	5.74	118.49	109.94
1	B	285	VAL	CB-CA-C	-5.74	106.34	111.74
1	C	166	ASP	O-C-N	5.74	127.98	122.07
1	B	62	ALA	CA-C-O	-5.74	113.62	120.10
1	B	166	ASP	O-C-N	5.74	127.98	122.07
1	C	50	LEU	CA-C-N	5.74	130.96	122.99
1	C	50	LEU	C-N-CA	5.74	130.96	122.99
1	C	330	THR	N-CA-CB	-5.73	100.80	110.49
1	D	260	ARG	N-CA-CB	5.73	118.48	109.94
1	A	48	ILE	CA-CB-CG2	5.72	120.23	110.50
1	A	313	ARG	CB-CA-C	5.72	121.04	110.56
1	D	48	ILE	CA-CB-CG2	5.72	120.23	110.50
1	D	138	ASN	CB-CG-ND2	5.72	124.99	116.40
1	D	330	THR	N-CA-CB	-5.72	100.81	110.49
1	A	330	THR	N-CA-CB	-5.72	100.82	110.49
1	B	313	ARG	CB-CA-C	5.72	121.03	110.56
1	B	330	THR	N-CA-CB	-5.71	100.84	110.49
1	C	48	ILE	CA-CB-CG2	5.71	120.21	110.50
1	D	63	MET	O-C-N	5.71	129.08	122.17
1	B	122	GLU	O-C-N	5.71	127.95	122.07
1	D	50	LEU	CA-C-N	5.71	130.92	122.99
1	D	50	LEU	C-N-CA	5.71	130.92	122.99
1	A	198	LEU	O-C-N	5.69	125.99	121.55
1	B	111	ASP	CA-C-O	-5.69	113.01	119.78
1	C	63	MET	O-C-N	5.69	129.06	122.17
1	A	285	VAL	CB-CA-C	-5.69	106.39	111.74
1	B	48	ILE	CA-CB-CG2	5.68	120.16	110.50
1	C	259	THR	N-CA-C	-5.68	105.09	111.28
1	A	111	ASP	OD1-CG-OD2	-5.67	109.28	122.90
1	B	111	ASP	OD1-CG-OD2	-5.66	109.31	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ILE	O-C-N	5.66	128.20	122.71
1	B	323	SER	CA-CB-OG	-5.66	99.78	111.10
1	B	169	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	A	323	SER	CA-CB-OG	-5.65	99.80	111.10
1	A	169	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	A	249	TYR	CB-CG-CD2	-5.64	112.34	120.80
1	B	93	VAL	CB-CA-C	5.64	117.79	110.96
1	B	249	TYR	CB-CG-CD2	-5.64	112.34	120.80
1	D	323	SER	CA-CB-OG	-5.64	99.83	111.10
1	A	111	ASP	CA-C-O	-5.63	113.08	119.78
1	D	249	TYR	CB-CG-CD2	-5.63	112.35	120.80
1	C	183	GLN	CA-C-N	5.63	132.17	122.09
1	C	183	GLN	C-N-CA	5.63	132.17	122.09
1	C	290	PRO	CA-C-O	-5.63	110.35	120.60
1	B	198	LEU	O-C-N	5.63	125.94	121.55
1	B	290	PRO	CA-C-O	-5.63	110.36	120.60
1	D	259	THR	N-CA-C	-5.62	105.15	111.28
1	C	29	GLY	CA-C-N	5.62	127.75	120.44
1	C	29	GLY	C-N-CA	5.62	127.75	120.44
1	C	323	SER	CA-CB-OG	-5.62	99.86	111.10
1	D	290	PRO	CA-C-O	-5.62	110.37	120.60
1	A	29	GLY	CA-C-N	5.62	127.74	120.44
1	A	29	GLY	C-N-CA	5.62	127.74	120.44
1	B	304	ILE	CB-CG1-CD1	-5.62	102.01	113.80
1	D	111	ASP	OD1-CG-OD2	-5.62	109.42	122.90
1	B	259	THR	N-CA-C	-5.61	105.16	111.28
1	D	169	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	A	290	PRO	CA-C-O	-5.61	110.39	120.60
1	C	111	ASP	CA-C-O	-5.61	113.11	119.78
1	D	277	ASP	OD1-CG-OD2	-5.60	109.46	122.90
1	A	183	GLN	CA-C-N	5.60	132.11	122.09
1	A	183	GLN	C-N-CA	5.60	132.11	122.09
1	C	277	ASP	OD1-CG-OD2	-5.60	109.47	122.90
1	B	183	GLN	CA-C-N	5.59	132.10	122.09
1	B	183	GLN	C-N-CA	5.59	132.10	122.09
1	C	111	ASP	OD1-CG-OD2	-5.59	109.47	122.90
1	C	206	ILE	O-C-N	5.59	128.14	122.71
1	A	304	ILE	CB-CG1-CD1	-5.59	102.05	113.80
1	B	29	GLY	CA-C-N	5.59	127.71	120.44
1	B	29	GLY	C-N-CA	5.59	127.71	120.44
1	C	254	GLY	CA-C-N	5.59	130.19	120.68
1	C	254	GLY	C-N-CA	5.59	130.19	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ASP	OD1-CG-OD2	-5.59	109.48	122.90
1	C	93	VAL	CB-CA-C	5.59	117.72	110.96
1	D	111	ASP	CA-C-O	-5.59	113.13	119.78
1	A	93	VAL	CB-CA-C	5.59	117.72	110.96
1	C	249	TYR	CB-CG-CD2	-5.59	112.42	120.80
1	C	304	ILE	CB-CG1-CD1	-5.59	102.07	113.80
1	D	29	GLY	CA-C-N	5.58	127.70	120.44
1	D	29	GLY	C-N-CA	5.58	127.70	120.44
1	A	206	ILE	O-C-N	5.58	128.12	122.71
1	A	277	ASP	OD1-CG-OD2	-5.58	109.51	122.90
1	B	254	GLY	CA-C-N	5.58	130.16	120.68
1	B	254	GLY	C-N-CA	5.58	130.16	120.68
1	A	230	PHE	CA-C-O	-5.57	114.51	120.42
1	D	304	ILE	CB-CG1-CD1	-5.57	102.10	113.80
1	B	51	ILE	O-C-N	5.57	129.21	123.20
1	A	259	THR	N-CA-C	-5.56	105.22	111.28
1	D	183	GLN	CA-C-N	5.56	132.04	122.09
1	D	183	GLN	C-N-CA	5.56	132.04	122.09
1	D	206	ILE	O-C-N	5.55	128.09	122.71
1	D	230	PHE	CA-C-O	-5.55	114.54	120.42
1	D	254	GLY	CA-C-N	5.55	130.11	120.68
1	D	254	GLY	C-N-CA	5.55	130.11	120.68
1	A	254	GLY	CA-C-N	5.54	130.10	120.68
1	A	254	GLY	C-N-CA	5.54	130.10	120.68
1	C	169	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	C	57	LYS	CD-CE-NZ	5.54	129.62	111.90
1	D	57	LYS	CD-CE-NZ	5.54	129.62	111.90
1	D	51	ILE	O-C-N	5.53	129.18	123.20
1	D	54	ASN	CA-CB-CG	5.53	118.13	112.60
1	B	57	LYS	CD-CE-NZ	5.53	129.59	111.90
1	A	144	THR	O-C-N	5.53	129.73	122.33
1	C	160	GLY	CA-C-O	5.53	125.25	120.94
1	C	51	ILE	O-C-N	5.52	129.16	123.20
1	D	169	ARG	N-CA-C	-5.52	105.17	111.07
1	B	160	GLY	CA-C-O	5.51	125.24	120.94
1	A	57	LYS	CD-CE-NZ	5.50	129.51	111.90
1	B	309	ASP	CB-CG-OD2	5.50	131.06	118.40
1	D	93	VAL	CB-CA-C	5.50	117.62	110.96
1	A	54	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	230	PHE	CA-C-O	-5.50	114.59	120.42
1	D	313	ARG	N-CA-C	-5.50	104.12	112.04
1	B	262	ILE	CB-CA-C	5.50	118.96	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	ASP	CB-CG-OD2	5.50	131.04	118.40
1	D	125	MET	N-CA-C	-5.50	104.70	111.40
1	C	125	MET	N-CA-C	-5.49	104.70	111.40
1	B	144	THR	O-C-N	5.49	129.69	122.33
1	A	262	ILE	CB-CA-C	5.48	118.94	111.87
1	C	54	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	313	ARG	N-CA-C	-5.48	104.15	112.04
1	B	40	MET	CG-SD-CE	-5.48	88.84	100.90
1	C	144	THR	O-C-N	5.48	129.67	122.33
1	A	75	PRO	CA-C-O	-5.47	110.64	120.60
1	B	313	ARG	N-CA-C	-5.47	104.16	112.04
1	B	75	PRO	CA-C-O	-5.47	110.64	120.60
1	A	40	MET	CG-SD-CE	-5.47	88.87	100.90
1	A	51	ILE	O-C-N	5.47	129.10	123.20
1	C	169	ARG	N-CA-C	-5.46	105.22	111.07
1	A	309	ASP	CB-CG-OD2	5.46	130.97	118.40
1	C	162	GLY	N-CA-C	5.46	121.18	111.73
1	A	160	GLY	CA-C-O	5.46	125.20	120.94
1	B	54	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	142	ILE	O-C-N	5.46	129.05	121.84
1	C	230	PHE	CA-C-O	-5.46	114.63	120.42
1	C	313	ARG	N-CA-C	-5.46	104.18	112.04
1	D	17	ASN	CA-C-N	5.46	131.97	121.54
1	D	17	ASN	C-N-CA	5.46	131.97	121.54
1	B	125	MET	N-CA-C	-5.46	104.74	111.40
1	C	40	MET	CG-SD-CE	-5.46	88.89	100.90
1	D	144	THR	O-C-N	5.46	129.65	122.33
1	D	309	ASP	CB-CG-OD2	5.46	130.96	118.40
1	A	142	ILE	O-C-N	5.45	129.04	121.84
1	B	162	GLY	N-CA-C	5.45	121.16	111.73
1	A	260	ARG	O-C-N	5.45	127.75	122.09
1	D	162	GLY	N-CA-C	5.45	121.15	111.73
1	A	16	LYS	CA-C-O	-5.44	114.78	117.94
1	A	162	GLY	N-CA-C	5.44	121.15	111.73
1	C	17	ASN	CA-C-N	5.44	131.92	121.54
1	C	17	ASN	C-N-CA	5.44	131.92	121.54
1	C	262	ILE	CB-CA-C	5.43	118.88	111.87
1	C	75	PRO	CA-C-O	-5.43	110.71	120.60
1	C	148	TRP	N-CA-C	-5.43	105.27	111.14
1	A	169	ARG	N-CA-C	-5.43	105.26	111.07
1	D	40	MET	CG-SD-CE	-5.43	88.95	100.90
1	A	17	ASN	CA-C-N	5.42	131.90	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ASN	C-N-CA	5.42	131.90	121.54
1	B	70	VAL	O-C-N	5.42	127.38	121.90
1	C	142	ILE	O-C-N	5.42	129.00	121.84
1	D	266	GLU	CA-CB-CG	5.42	124.95	114.10
1	A	70	VAL	O-C-N	5.42	127.38	121.90
1	D	262	ILE	CB-CA-C	5.42	118.87	111.87
1	C	266	GLU	CA-CB-CG	5.42	124.94	114.10
1	D	142	ILE	O-C-N	5.42	129.00	121.84
1	A	148	TRP	N-CA-C	-5.42	105.29	111.14
1	B	260	ARG	O-C-N	5.42	127.72	122.09
1	D	75	PRO	CA-C-O	-5.42	110.74	120.60
1	B	169	ARG	N-CA-C	-5.41	105.28	111.07
1	C	271	THR	CA-C-N	5.41	131.71	121.97
1	C	271	THR	C-N-CA	5.41	131.71	121.97
1	A	266	GLU	CA-CB-CG	5.41	124.92	114.10
1	B	271	THR	CA-C-N	5.41	131.71	121.97
1	B	271	THR	C-N-CA	5.41	131.71	121.97
1	B	266	GLU	CA-CB-CG	5.41	124.92	114.10
1	B	87	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	C	47	GLU	CG-CD-OE2	-5.40	105.98	118.40
1	C	260	ARG	O-C-N	5.40	127.71	122.09
1	B	17	ASN	CA-C-N	5.40	131.85	121.54
1	B	17	ASN	C-N-CA	5.40	131.85	121.54
1	A	125	MET	N-CA-C	-5.40	104.82	111.40
1	B	91	LEU	N-CA-CB	-5.40	101.75	110.71
1	A	271	THR	CA-C-N	5.39	131.68	121.97
1	A	271	THR	C-N-CA	5.39	131.68	121.97
1	B	253	MET	N-CA-C	-5.39	105.40	111.28
1	D	47	GLU	CG-CD-OE2	-5.39	106.00	118.40
1	B	47	GLU	CG-CD-OE2	-5.39	106.00	118.40
1	C	63	MET	N-CA-C	-5.39	104.82	111.40
1	D	260	ARG	O-C-N	5.39	127.70	122.09
1	A	139	PRO	CA-C-O	-5.39	107.26	120.20
1	B	139	PRO	CA-C-O	-5.39	107.27	120.20
1	A	91	LEU	N-CA-CB	-5.38	101.77	110.71
1	B	148	TRP	N-CA-C	-5.38	105.33	111.14
1	C	198	LEU	CA-C-O	-5.38	115.31	120.64
1	D	91	LEU	N-CA-CB	-5.38	101.78	110.71
1	D	139	PRO	CA-C-O	-5.38	107.29	120.20
1	C	139	PRO	CA-C-O	-5.37	107.30	120.20
1	D	271	THR	CA-C-N	5.37	131.64	121.97
1	D	271	THR	C-N-CA	5.37	131.64	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	VAL	CB-CA-C	5.37	119.63	112.22
1	D	160	GLY	CA-C-O	5.37	125.13	120.94
1	D	225	ASP	CA-C-N	5.37	131.21	121.92
1	D	225	ASP	C-N-CA	5.37	131.21	121.92
1	D	70	VAL	O-C-N	5.37	127.32	121.90
1	A	47	GLU	CG-CD-OE2	-5.36	106.06	118.40
1	A	307	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	225	ASP	CA-C-N	5.36	131.19	121.92
1	B	225	ASP	C-N-CA	5.36	131.19	121.92
1	C	91	LEU	N-CA-CB	-5.36	101.82	110.71
1	C	31	VAL	CB-CA-C	5.35	119.61	112.22
1	C	225	ASP	CA-C-N	5.35	131.18	121.92
1	C	225	ASP	C-N-CA	5.35	131.18	121.92
1	A	31	VAL	CB-CA-C	5.35	119.61	112.22
1	A	253	MET	N-CA-C	-5.35	105.45	111.28
1	D	63	MET	N-CA-C	-5.35	104.87	111.40
1	A	288	GLY	O-C-N	5.35	129.66	122.70
1	D	148	TRP	N-CA-C	-5.35	105.36	111.14
1	A	225	ASP	CA-C-N	5.35	131.17	121.92
1	A	225	ASP	C-N-CA	5.35	131.17	121.92
1	A	63	MET	N-CA-C	-5.34	104.88	111.40
1	B	63	MET	N-CA-C	-5.34	104.88	111.40
1	C	87	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	B	247	THR	CA-CB-CG2	5.33	119.57	110.50
1	C	307	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	288	GLY	O-C-N	5.33	129.63	122.70
1	C	253	MET	N-CA-C	-5.33	105.47	111.28
1	D	307	ASN	CA-CB-CG	5.32	117.92	112.60
1	D	198	LEU	CA-C-O	-5.32	115.38	120.64
1	A	247	THR	CA-CB-CG2	5.31	119.53	110.50
1	B	178	PHE	CA-C-O	5.31	125.90	119.11
1	B	277	ASP	N-CA-CB	-5.30	101.58	110.39
1	C	247	THR	CA-CB-CG2	5.30	119.52	110.50
1	D	189	ILE	O-C-N	-5.30	117.58	123.20
1	D	31	VAL	CB-CA-C	5.30	119.54	112.22
1	C	17	ASN	CB-CA-C	5.30	119.27	110.74
1	C	70	VAL	O-C-N	5.30	127.25	121.90
1	D	17	ASN	CB-CA-C	5.30	119.27	110.74
1	A	172	PHE	CA-C-O	-5.29	112.94	120.51
1	B	172	PHE	CA-C-O	-5.29	112.95	120.51
1	D	87	ARG	NE-CZ-NH1	5.29	126.79	121.50
1	D	288	GLY	O-C-N	5.29	129.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247	THR	CA-CB-CG2	5.28	119.48	110.50
1	A	277	ASP	N-CA-CB	-5.28	101.63	110.39
1	B	16	LYS	CA-C-O	-5.28	114.88	117.94
1	C	189	ILE	O-C-N	-5.28	117.60	123.20
1	C	277	ASP	N-CA-CB	-5.28	101.63	110.39
1	C	288	GLY	O-C-N	5.28	129.56	122.70
1	D	277	ASP	N-CA-CB	-5.28	101.63	110.39
1	A	87	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	B	307	ASN	CA-CB-CG	5.28	117.88	112.60
1	D	276	LEU	CB-CA-C	5.28	119.03	110.22
1	D	253	MET	N-CA-C	-5.28	105.53	111.28
1	B	17	ASN	CB-CA-C	5.27	119.23	110.74
1	D	16	LYS	CA-C-O	-5.27	114.88	117.94
1	A	178	PHE	CA-C-O	5.27	125.85	119.11
1	B	198	LEU	CA-C-O	-5.27	115.42	120.64
1	C	276	LEU	CB-CA-C	5.26	119.01	110.22
1	D	172	PHE	CA-C-O	-5.26	112.99	120.51
1	C	178	PHE	CA-C-O	5.26	125.84	119.11
1	A	198	LEU	CA-C-O	-5.26	115.44	120.64
1	D	190	ILE	CA-C-O	-5.26	116.31	121.67
1	A	17	ASN	CB-CA-C	5.25	119.20	110.74
1	A	276	LEU	CB-CA-C	5.25	118.99	110.22
1	A	324	VAL	CB-CA-C	-5.25	103.76	112.26
1	C	172	PHE	CA-C-O	-5.25	113.01	120.51
1	B	189	ILE	O-C-N	-5.25	117.64	123.20
1	B	276	LEU	CB-CA-C	5.24	118.98	110.22
1	D	178	PHE	CA-C-O	5.24	125.82	119.11
1	D	154	PRO	N-CA-C	-5.23	102.79	111.11
1	C	16	LYS	CA-C-O	-5.23	114.91	117.94
1	B	299	ARG	CA-C-O	5.22	126.84	120.31
1	A	52	ASP	CB-CG-OD1	5.21	130.39	118.40
1	C	190	ILE	CA-C-O	-5.21	116.35	121.67
1	B	190	ILE	CA-C-O	-5.21	116.36	121.67
1	B	324	VAL	CB-CA-C	-5.21	103.82	112.26
1	C	154	PRO	N-CA-C	-5.21	102.83	111.11
1	C	324	VAL	CB-CA-C	-5.21	103.83	112.26
1	A	189	ILE	O-C-N	-5.21	117.68	123.20
1	C	299	ARG	CA-C-O	5.21	126.82	120.31
1	C	138	ASN	O-C-N	-5.20	115.61	121.43
1	A	154	PRO	N-CA-C	-5.20	102.85	111.11
1	B	138	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	154	PRO	N-CA-C	-5.19	102.85	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	299	ARG	CA-C-O	5.19	126.80	120.31
1	A	190	ILE	CA-C-O	-5.19	116.38	121.67
1	A	25	VAL	CA-C-O	-5.18	114.94	120.59
1	B	52	ASP	CB-CG-OD1	5.18	130.32	118.40
1	A	138	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	299	ARG	CA-C-O	5.18	126.78	120.31
1	B	25	VAL	CA-C-O	-5.18	114.94	120.59
1	B	262	ILE	N-CA-C	-5.18	105.55	110.42
1	D	52	ASP	CB-CG-OD1	5.17	130.30	118.40
1	B	138	ASN	O-C-N	-5.17	115.64	121.43
1	D	324	VAL	CB-CA-C	-5.17	103.89	112.26
1	B	297	GLY	CA-C-O	-5.17	111.58	120.57
1	A	297	GLY	CA-C-O	-5.16	111.59	120.57
1	C	52	ASP	CB-CG-OD1	5.16	130.27	118.40
1	A	266	GLU	N-CA-CB	5.16	117.55	110.07
1	D	297	GLY	CA-C-O	-5.16	111.60	120.57
1	D	138	ASN	O-C-N	-5.15	115.66	121.43
1	B	266	GLU	N-CA-CB	5.13	117.52	110.07
1	A	138	ASN	O-C-N	-5.13	115.68	121.43
1	C	25	VAL	CA-C-O	-5.13	115.00	120.59
1	B	228	ARG	N-CA-C	-5.13	104.62	111.24
1	A	313	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	C	89	ALA	CA-C-N	5.12	127.14	120.28
1	C	89	ALA	C-N-CA	5.12	127.14	120.28
1	C	262	ILE	N-CA-C	-5.12	105.60	110.42
1	D	69	LYS	O-C-N	5.12	127.55	122.12
1	D	255	LEU	CA-C-O	5.12	125.83	119.79
1	D	266	GLU	N-CA-CB	5.12	117.50	110.07
1	A	255	LEU	CA-C-O	5.12	125.83	119.79
1	B	151	SER	CA-CB-OG	-5.11	100.87	111.10
1	C	297	GLY	CA-C-O	-5.11	111.67	120.57
1	A	69	LYS	O-C-N	5.11	127.54	122.12
1	C	138	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	D	277	ASP	N-CA-C	5.11	118.78	112.54
1	C	69	LYS	O-C-N	5.11	127.54	122.12
1	C	266	GLU	N-CA-CB	5.11	117.48	110.07
1	D	94	ILE	CA-C-N	5.11	130.83	122.65
1	D	94	ILE	C-N-CA	5.11	130.83	122.65
1	D	313	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	151	SER	CA-CB-OG	-5.11	100.89	111.10
1	A	89	ALA	CA-C-N	5.11	127.12	120.28
1	A	89	ALA	C-N-CA	5.11	127.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ALA	CA-C-O	5.11	125.84	119.97
1	A	90	ASP	N-CA-C	5.10	116.84	111.28
1	A	228	ARG	N-CA-C	-5.10	104.66	111.24
1	C	277	ASP	N-CA-C	5.10	118.76	112.54
1	D	228	ARG	N-CA-C	-5.10	104.67	111.24
1	D	89	ALA	CA-C-N	5.09	127.11	120.28
1	D	89	ALA	C-N-CA	5.09	127.11	120.28
1	A	94	ILE	CA-C-N	5.09	130.79	122.65
1	A	94	ILE	C-N-CA	5.09	130.79	122.65
1	A	286	TYR	N-CA-C	-5.09	100.60	108.90
1	D	90	ASP	N-CA-C	5.08	116.82	111.28
1	C	94	ILE	CA-C-N	5.08	130.78	122.65
1	C	94	ILE	C-N-CA	5.08	130.78	122.65
1	D	25	VAL	CA-C-O	-5.08	115.05	120.59
1	B	90	ASP	N-CA-C	5.08	116.81	111.28
1	C	146	ALA	CA-C-O	5.08	125.81	119.97
1	B	89	ALA	CA-C-N	5.07	127.08	120.28
1	B	89	ALA	C-N-CA	5.07	127.08	120.28
1	D	151	SER	CA-CB-OG	-5.07	100.95	111.10
1	C	90	ASP	N-CA-C	5.07	116.81	111.28
1	B	286	TYR	N-CA-C	-5.07	100.64	108.90
1	D	195	ASP	N-CA-C	5.07	116.89	111.36
1	C	151	SER	CA-CB-OG	-5.07	100.96	111.10
1	C	286	TYR	N-CA-C	-5.07	100.64	108.90
1	A	262	ILE	N-CA-C	-5.07	105.66	110.42
1	C	255	LEU	CA-C-O	5.07	125.77	119.79
1	B	124	VAL	O-C-N	5.06	129.11	122.12
1	C	77	ASP	CB-CG-OD2	-5.06	106.76	118.40
1	C	195	ASP	N-CA-C	5.06	116.88	111.36
1	B	94	ILE	CA-C-N	5.06	130.74	122.65
1	B	94	ILE	C-N-CA	5.06	130.74	122.65
1	B	195	ASP	N-CA-C	5.06	116.88	111.36
1	B	207	GLY	N-CA-C	-5.06	101.19	113.18
1	B	313	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	C	124	VAL	O-C-N	5.06	129.10	122.12
1	D	146	ALA	CA-C-O	5.06	125.79	119.97
1	B	69	LYS	O-C-N	5.06	127.48	122.12
1	B	255	LEU	CA-C-O	5.05	125.75	119.79
1	B	309	ASP	CA-C-O	5.05	125.79	119.78
1	C	309	ASP	CA-C-O	5.05	125.79	119.78
1	A	207	GLY	N-CA-C	-5.05	101.22	113.18
1	B	146	ALA	CA-C-O	5.05	125.78	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	TYR	N-CA-C	-5.05	100.67	108.90
1	B	77	ASP	CB-CG-OD2	-5.05	106.79	118.40
1	C	116	ILE	CA-C-O	-5.05	115.45	121.05
1	D	262	ILE	N-CA-C	-5.05	105.68	110.42
1	A	124	VAL	O-C-N	5.04	129.08	122.12
1	C	228	ARG	N-CA-C	-5.04	104.74	111.24
1	D	176	GLU	CB-CG-CD	5.04	121.17	112.60
1	D	124	VAL	O-C-N	5.04	129.07	122.12
1	D	77	ASP	CB-CG-OD2	-5.03	106.83	118.40
1	D	138	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	309	ASP	CA-C-O	5.03	125.77	119.78
1	D	26	ILE	CB-CA-C	5.03	117.63	111.25
1	D	267	ASN	N-CA-CB	5.03	118.98	110.49
1	C	176	GLU	CB-CG-CD	5.02	121.14	112.60
1	C	313	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	77	ASP	CB-CG-OD2	-5.02	106.85	118.40
1	B	277	ASP	N-CA-C	5.02	118.67	112.54
1	D	309	ASP	CA-C-O	5.02	125.76	119.78
1	C	207	GLY	N-CA-C	-5.02	101.29	113.18
1	D	207	GLY	N-CA-C	-5.02	101.29	113.18
1	C	267	ASN	N-CA-CB	5.01	118.96	110.49
1	C	112	LYS	O-C-N	5.01	129.65	122.13
1	B	130	GLN	CB-CA-C	-5.01	100.65	109.07
1	B	176	GLU	CB-CG-CD	5.01	121.12	112.60
1	B	303	GLU	N-CA-CB	5.01	117.85	110.49
1	C	307	ASN	N-CA-C	-5.00	100.14	110.80
1	C	303	GLU	N-CA-CB	5.00	117.84	110.49
1	C	303	GLU	CB-CA-C	-5.00	104.45	112.05

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Mainchain
1	A	134	LEU	Mainchain
1	A	147	THR	Mainchain
1	A	152	GLY	Mainchain
1	A	154	PRO	Mainchain
1	A	167	THR	Mainchain
1	A	170	PHE	Sidechain
1	A	171	ARG	Sidechain
1	A	184	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	188	TYR	Mainchain
1	A	191	GLY	Mainchain
1	A	206	ILE	Mainchain
1	A	207	GLY	Mainchain
1	A	229	ILE	Mainchain
1	A	23	VAL	Mainchain
1	A	275	TYR	Sidechain
1	A	281	GLY	Mainchain
1	A	285	VAL	Mainchain
1	A	286	TYR	Sidechain
1	A	295	ARG	Mainchain
1	A	30	PHE	Sidechain
1	A	300	GLU	Mainchain
1	A	301	VAL	Mainchain
1	A	310	GLU	Mainchain
1	A	312	ASN	Mainchain
1	A	323	SER	Mainchain
1	A	325	LEU	Mainchain
1	A	49	VAL	Mainchain
1	A	62	ALA	Mainchain
1	A	77	ASP	Mainchain
1	A	94	ILE	Mainchain
1	B	111	ASP	Mainchain
1	B	134	LEU	Mainchain
1	B	147	THR	Mainchain
1	B	152	GLY	Mainchain
1	B	154	PRO	Mainchain
1	B	167	THR	Mainchain
1	B	170	PHE	Sidechain
1	B	171	ARG	Sidechain
1	B	184	ASN	Mainchain
1	B	188	TYR	Mainchain
1	B	191	GLY	Mainchain
1	B	206	ILE	Mainchain
1	B	207	GLY	Mainchain
1	B	229	ILE	Mainchain
1	B	23	VAL	Mainchain
1	B	275	TYR	Sidechain
1	B	281	GLY	Mainchain
1	B	285	VAL	Mainchain
1	B	286	TYR	Sidechain
1	B	295	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	B	30	PHE	Sidechain
1	B	300	GLU	Mainchain
1	B	301	VAL	Mainchain
1	B	310	GLU	Mainchain
1	B	312	ASN	Mainchain
1	B	323	SER	Mainchain
1	B	325	LEU	Mainchain
1	B	326	ALA	Mainchain
1	B	49	VAL	Mainchain
1	B	62	ALA	Mainchain
1	B	77	ASP	Mainchain
1	B	94	ILE	Mainchain
1	C	111	ASP	Mainchain
1	C	134	LEU	Mainchain
1	C	147	THR	Mainchain
1	C	152	GLY	Mainchain
1	C	154	PRO	Mainchain
1	C	167	THR	Mainchain
1	C	170	PHE	Sidechain
1	C	171	ARG	Sidechain
1	C	184	ASN	Mainchain
1	C	188	TYR	Mainchain
1	C	191	GLY	Mainchain
1	C	206	ILE	Mainchain
1	C	207	GLY	Mainchain
1	C	229	ILE	Mainchain
1	C	23	VAL	Mainchain
1	C	275	TYR	Sidechain
1	C	281	GLY	Mainchain
1	C	285	VAL	Mainchain
1	C	286	TYR	Sidechain
1	C	295	ARG	Mainchain
1	C	30	PHE	Sidechain
1	C	300	GLU	Mainchain
1	C	301	VAL	Mainchain
1	C	310	GLU	Mainchain
1	C	312	ASN	Mainchain
1	C	323	SER	Mainchain
1	C	325	LEU	Mainchain
1	C	49	VAL	Mainchain
1	C	62	ALA	Mainchain
1	C	77	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	C	94	ILE	Mainchain
1	D	111	ASP	Mainchain
1	D	134	LEU	Mainchain
1	D	147	THR	Mainchain
1	D	152	GLY	Mainchain
1	D	154	PRO	Mainchain
1	D	167	THR	Mainchain
1	D	170	PHE	Sidechain
1	D	171	ARG	Sidechain
1	D	184	ASN	Mainchain
1	D	188	TYR	Mainchain
1	D	191	GLY	Mainchain
1	D	206	ILE	Mainchain
1	D	207	GLY	Mainchain
1	D	229	ILE	Mainchain
1	D	23	VAL	Mainchain
1	D	275	TYR	Sidechain
1	D	281	GLY	Mainchain
1	D	285	VAL	Mainchain
1	D	286	TYR	Sidechain
1	D	295	ARG	Mainchain
1	D	30	PHE	Sidechain
1	D	300	GLU	Mainchain
1	D	301	VAL	Mainchain
1	D	310	GLU	Mainchain
1	D	312	ASN	Mainchain
1	D	323	SER	Mainchain
1	D	325	LEU	Mainchain
1	D	49	VAL	Mainchain
1	D	62	ALA	Mainchain
1	D	77	ASP	Mainchain
1	D	94	ILE	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	2277	0	2253	217	46

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2277	0	2253	216	0
1	C	2277	0	2253	221	11
1	D	2277	0	2253	214	57
2	A	10	0	0	2	0
3	A	1	0	0	1	0
All	All	9119	0	9012	803	57

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 44.

All (803) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HG3	1:D:88:ASP:H	1.12	1.13
1:B:87:ARG:HG3	1:B:88:ASP:H	1.11	1.12
1:D:142:ILE:HD13	1:D:324:VAL:HG11	1.31	1.11
1:C:142:ILE:HD13	1:C:324:VAL:HG11	1.31	1.10
1:B:142:ILE:HD13	1:B:324:VAL:HG11	1.32	1.09
1:B:265:ASN:HD22	1:B:295:ARG:HB2	1.18	1.09
1:C:265:ASN:HD22	1:C:295:ARG:HB2	1.18	1.08
1:A:87:ARG:HG3	1:A:88:ASP:H	1.11	1.08
1:C:87:ARG:HG3	1:C:88:ASP:H	1.11	1.07
1:A:265:ASN:HD22	1:A:295:ARG:HB2	1.18	1.06
1:D:265:ASN:HD22	1:D:295:ARG:HB2	1.18	1.06
1:A:142:ILE:HD13	1:A:324:VAL:HG11	1.32	1.06
1:B:311:LYS:HA	1:B:315:HIS:HB2	1.40	1.03
1:A:311:LYS:HA	1:A:315:HIS:HB2	1.40	1.03
1:A:310:GLU:O	1:A:312:ASN:N	1.93	1.02
1:B:18:ASN:HD22	1:B:18:ASN:N	1.50	1.02
1:D:18:ASN:N	1:D:18:ASN:HD22	1.50	1.02
1:C:311:LYS:HA	1:C:315:HIS:HB2	1.41	1.02
1:D:18:ASN:H	1:D:18:ASN:ND2	1.53	1.02
1:B:310:GLU:O	1:B:312:ASN:N	1.93	1.01
1:C:310:GLU:O	1:C:312:ASN:N	1.93	1.00
1:D:310:GLU:O	1:D:312:ASN:N	1.93	1.00
1:B:18:ASN:ND2	1:B:18:ASN:H	1.53	1.00
1:A:18:ASN:H	1:A:18:ASN:ND2	1.53	1.00
1:C:18:ASN:N	1:C:18:ASN:HD22	1.49	1.00
1:D:311:LYS:HA	1:D:315:HIS:HB2	1.40	0.99
1:C:18:ASN:H	1:C:18:ASN:ND2	1.52	0.97
1:A:18:ASN:N	1:A:18:ASN:HD22	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:CG	1:A:88:ASP:H	1.77	0.94
1:B:87:ARG:CG	1:B:88:ASP:H	1.77	0.93
1:A:265:ASN:ND2	1:A:295:ARG:HB2	1.84	0.93
1:D:265:ASN:ND2	1:D:295:ARG:HB2	1.84	0.93
1:C:265:ASN:ND2	1:C:295:ARG:HB2	1.84	0.92
1:B:265:ASN:ND2	1:B:295:ARG:HB2	1.84	0.92
1:C:87:ARG:CG	1:C:88:ASP:H	1.77	0.92
1:C:87:ARG:HG3	1:C:88:ASP:N	1.86	0.91
1:B:87:ARG:HG3	1:B:88:ASP:N	1.86	0.90
1:A:87:ARG:HG3	1:A:88:ASP:N	1.86	0.88
1:A:142:ILE:CD1	1:A:324:VAL:HG11	2.04	0.88
1:C:87:ARG:NH1	1:C:87:ARG:HB2	1.89	0.88
1:B:87:ARG:HB2	1:B:87:ARG:NH1	1.89	0.88
1:C:200:VAL:HG11	1:C:304:ILE:HD12	1.56	0.87
1:D:87:ARG:CG	1:D:88:ASP:H	1.77	0.87
1:D:200:VAL:HG11	1:D:304:ILE:HD12	1.56	0.87
1:D:142:ILE:CD1	1:D:324:VAL:HG11	2.04	0.87
1:B:142:ILE:CD1	1:B:324:VAL:HG11	2.04	0.87
1:C:142:ILE:CD1	1:C:324:VAL:HG11	2.04	0.87
1:A:182:PRO:HB2	1:C:70:VAL:HG22	1.57	0.86
1:B:182:PRO:HB2	1:D:70:VAL:HG22	1.57	0.86
1:A:87:ARG:NH1	1:A:87:ARG:HB2	1.89	0.86
1:B:70:VAL:HG22	1:D:182:PRO:HB2	1.57	0.86
1:D:295:ARG:HG3	1:D:295:ARG:HH11	1.40	0.86
1:B:200:VAL:HG11	1:B:304:ILE:HD12	1.56	0.85
1:D:87:ARG:HB2	1:D:87:ARG:NH1	1.89	0.85
1:A:295:ARG:HG3	1:A:295:ARG:HH11	1.40	0.85
1:B:244:LYS:HG2	1:B:244:LYS:O	1.77	0.85
1:C:295:ARG:HG3	1:C:295:ARG:HH11	1.40	0.85
1:A:200:VAL:HG11	1:A:304:ILE:HD12	1.57	0.85
1:A:311:LYS:HA	1:A:315:HIS:CB	2.07	0.85
1:A:70:VAL:HG22	1:C:182:PRO:HB2	1.58	0.85
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.40	0.84
1:D:87:ARG:HG3	1:D:88:ASP:N	1.86	0.84
1:A:244:LYS:O	1:A:244:LYS:HG2	1.77	0.84
1:C:109:LEU:O	1:C:113:ASN:HB2	1.78	0.84
1:B:55:GLU:O	1:B:59:ILE:HD12	1.78	0.84
1:B:311:LYS:HA	1:B:315:HIS:CB	2.07	0.84
1:D:311:LYS:HA	1:D:315:HIS:CB	2.07	0.83
1:D:109:LEU:O	1:D:113:ASN:HB2	1.78	0.83
1:B:109:LEU:O	1:B:113:ASN:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLU:O	1:D:59:ILE:HD12	1.78	0.83
1:A:55:GLU:O	1:A:59:ILE:HD12	1.78	0.83
1:A:109:LEU:O	1:A:113:ASN:HB2	1.78	0.83
1:C:311:LYS:HA	1:C:315:HIS:CB	2.07	0.83
1:C:55:GLU:O	1:C:59:ILE:HD12	1.78	0.82
1:C:200:VAL:HG11	1:C:304:ILE:CD1	2.10	0.82
1:D:328:ALA:O	1:D:329:PHE:HB2	1.80	0.82
1:C:244:LYS:O	1:C:244:LYS:HG2	1.77	0.81
1:D:200:VAL:HG11	1:D:304:ILE:CD1	2.11	0.81
1:B:200:VAL:HG11	1:B:304:ILE:CD1	2.10	0.81
1:D:310:GLU:C	1:D:312:ASN:H	1.89	0.81
1:D:244:LYS:O	1:D:244:LYS:HG2	1.77	0.81
1:C:310:GLU:C	1:C:312:ASN:H	1.89	0.81
1:A:328:ALA:O	1:A:329:PHE:HB2	1.81	0.80
1:C:328:ALA:O	1:C:329:PHE:HB2	1.80	0.80
1:C:240:ILE:CG1	1:C:247:THR:HG22	2.12	0.80
1:B:328:ALA:O	1:B:329:PHE:HB2	1.80	0.80
1:A:310:GLU:C	1:A:312:ASN:H	1.89	0.80
1:B:270:LEU:HD12	1:B:293:ILE:HD12	1.64	0.80
1:A:130:GLN:O	1:A:157:ARG:NH1	2.15	0.80
1:A:270:LEU:HD12	1:A:293:ILE:HD12	1.64	0.80
1:B:163:THR:O	1:B:167:THR:HG23	1.82	0.80
1:B:240:ILE:CG1	1:B:247:THR:HG22	2.12	0.80
1:D:240:ILE:CG1	1:D:247:THR:HG22	2.12	0.80
1:B:310:GLU:C	1:B:312:ASN:H	1.89	0.79
1:A:200:VAL:HG11	1:A:304:ILE:CD1	2.11	0.79
1:A:163:THR:O	1:A:167:THR:HG23	1.82	0.79
1:B:178:PHE:CE1	1:B:206:ILE:CD1	2.66	0.79
1:A:240:ILE:CG1	1:A:247:THR:HG22	2.12	0.79
1:B:130:GLN:O	1:B:157:ARG:NH1	2.15	0.79
1:B:244:LYS:HE3	1:D:61:ASP:OD1	1.83	0.79
1:D:130:GLN:O	1:D:157:ARG:NH1	2.15	0.79
1:C:130:GLN:O	1:C:157:ARG:NH1	2.15	0.79
1:D:178:PHE:CE1	1:D:206:ILE:CD1	2.66	0.79
1:A:61:ASP:OD1	1:C:244:LYS:HE3	1.83	0.78
1:D:163:THR:O	1:D:167:THR:HG23	1.83	0.78
1:A:178:PHE:CE1	1:A:206:ILE:CD1	2.66	0.78
1:A:244:LYS:HE3	1:C:61:ASP:OD1	1.83	0.78
1:B:61:ASP:OD1	1:D:244:LYS:HE3	1.83	0.78
1:C:178:PHE:CE1	1:C:206:ILE:CD1	2.66	0.78
1:C:270:LEU:HD12	1:C:293:ILE:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:O	1:C:167:THR:HG23	1.83	0.78
1:D:270:LEU:HD12	1:D:293:ILE:HD12	1.64	0.77
1:C:310:GLU:C	1:C:312:ASN:N	2.41	0.76
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.18	0.75
1:A:178:PHE:CE1	1:A:206:ILE:HD11	2.22	0.74
1:B:178:PHE:CE1	1:B:206:ILE:HD11	2.22	0.74
1:C:178:PHE:CE1	1:C:206:ILE:HD11	2.22	0.74
1:B:18:ASN:HD22	1:B:18:ASN:H	0.77	0.74
1:D:178:PHE:CE1	1:D:206:ILE:HD11	2.22	0.74
1:B:15:MET:CE	1:B:18:ASN:HA	2.18	0.74
1:C:257:ARG:NH2	1:C:266:GLU:OE2	2.18	0.73
1:D:306:LEU:O	1:D:307:ASN:O	2.06	0.73
1:C:306:LEU:O	1:C:307:ASN:O	2.06	0.73
1:D:257:ARG:NH2	1:D:266:GLU:OE2	2.18	0.73
1:C:15:MET:CE	1:C:18:ASN:HA	2.18	0.73
1:B:306:LEU:O	1:B:307:ASN:O	2.06	0.73
1:B:310:GLU:C	1:B:312:ASN:N	2.42	0.73
1:A:306:LEU:O	1:A:307:ASN:O	2.06	0.73
1:C:55:GLU:HG3	1:C:59:ILE:HD11	1.71	0.73
1:A:15:MET:CE	1:A:18:ASN:HA	2.19	0.73
1:A:310:GLU:C	1:A:312:ASN:N	2.41	0.73
1:D:83:TYR:C	1:D:85:ASP:H	1.96	0.73
1:D:15:MET:CE	1:D:18:ASN:HA	2.18	0.72
1:C:87:ARG:HB2	1:C:87:ARG:CZ	2.20	0.72
1:D:87:ARG:HB2	1:D:87:ARG:CZ	2.20	0.72
1:A:118:ARG:O	1:A:122:GLU:HG2	1.90	0.72
1:B:83:TYR:C	1:B:85:ASP:H	1.97	0.71
1:C:83:TYR:C	1:C:85:ASP:H	1.96	0.71
1:B:87:ARG:HB2	1:B:87:ARG:CZ	2.20	0.71
1:A:55:GLU:HG3	1:A:59:ILE:HD11	1.71	0.71
1:C:24:VAL:HG22	1:C:49:VAL:HB	1.73	0.71
1:D:55:GLU:HG3	1:D:59:ILE:HD11	1.71	0.71
1:A:86:CYS:HA	1:A:89:ALA:CB	2.21	0.71
1:B:24:VAL:HG22	1:B:49:VAL:HB	1.73	0.71
1:B:118:ARG:O	1:B:122:GLU:HG2	1.90	0.71
1:D:18:ASN:HD22	1:D:18:ASN:H	0.77	0.71
1:D:118:ARG:O	1:D:122:GLU:HG2	1.90	0.71
1:C:86:CYS:HA	1:C:89:ALA:CB	2.21	0.70
1:A:83:TYR:C	1:A:85:ASP:H	1.96	0.70
1:B:55:GLU:HG3	1:B:59:ILE:HD11	1.71	0.70
1:B:86:CYS:HA	1:B:89:ALA:CB	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HG22	1:B:189:ILE:H	1.56	0.70
1:C:118:ARG:O	1:C:122:GLU:HG2	1.90	0.70
1:D:310:GLU:C	1:D:312:ASN:N	2.41	0.70
1:B:283:ARG:H	1:B:322:LYS:NZ	1.90	0.70
1:D:68:GLY:O	1:D:71:PHE:HB2	1.91	0.70
1:A:68:GLY:O	1:A:71:PHE:HB2	1.91	0.70
1:C:68:GLY:O	1:C:71:PHE:HB2	1.92	0.70
1:D:283:ARG:H	1:D:322:LYS:NZ	1.90	0.70
1:A:283:ARG:H	1:A:322:LYS:NZ	1.90	0.70
1:D:86:CYS:HA	1:D:89:ALA:CB	2.21	0.70
1:A:167:THR:HG22	1:A:189:ILE:H	1.56	0.69
1:A:257:ARG:NH2	1:A:266:GLU:OE2	2.18	0.69
1:B:68:GLY:O	1:B:71:PHE:HB2	1.91	0.69
1:A:24:VAL:HG22	1:A:49:VAL:HB	1.73	0.69
1:C:167:THR:HG22	1:C:189:ILE:H	1.57	0.69
1:C:283:ARG:H	1:C:322:LYS:NZ	1.90	0.69
1:D:167:THR:HG22	1:D:189:ILE:H	1.56	0.69
1:A:87:ARG:HB2	1:A:87:ARG:CZ	2.20	0.69
1:A:279:LEU:HD23	1:A:301:VAL:CG1	2.22	0.69
1:B:279:LEU:HD23	1:B:301:VAL:CG1	2.22	0.69
1:C:279:LEU:HD23	1:C:301:VAL:CG1	2.22	0.69
1:D:24:VAL:HG22	1:D:49:VAL:HB	1.73	0.69
1:D:279:LEU:HD23	1:D:301:VAL:CG1	2.22	0.69
1:B:189:ILE:CD1	1:B:233:VAL:HG11	2.23	0.69
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.23	0.69
1:A:189:ILE:CD1	1:A:233:VAL:HG11	2.23	0.68
1:D:189:ILE:CG2	1:D:197:GLU:HG3	2.24	0.68
1:D:189:ILE:CD1	1:D:233:VAL:HG11	2.24	0.68
1:C:18:ASN:HD22	1:C:18:ASN:H	0.77	0.67
1:A:189:ILE:CG2	1:A:197:GLU:HG3	2.24	0.67
1:C:189:ILE:CG2	1:C:197:GLU:HG3	2.24	0.67
1:B:189:ILE:CG2	1:B:197:GLU:HG3	2.24	0.67
1:D:257:ARG:NH1	1:D:257:ARG:HG3	2.10	0.67
1:A:18:ASN:H	1:A:18:ASN:HD22	0.77	0.66
1:D:18:ASN:N	1:D:18:ASN:ND2	2.24	0.66
1:C:257:ARG:HG3	1:C:257:ARG:HH11	1.61	0.66
1:C:257:ARG:HG3	1:C:257:ARG:NH1	2.10	0.66
1:D:265:ASN:ND2	1:D:295:ARG:CB	2.60	0.65
1:A:142:ILE:HD13	1:A:324:VAL:CG1	2.20	0.65
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.62	0.65
1:B:257:ARG:NH1	1:B:257:ARG:HG3	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:ND2	1:A:18:ASN:N	2.24	0.65
1:B:257:ARG:HG3	1:B:257:ARG:HH11	1.61	0.65
1:D:110:VAL:O	1:D:114:ILE:HG13	1.97	0.65
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.10	0.65
1:C:265:ASN:ND2	1:C:295:ARG:CB	2.60	0.65
1:B:42:GLN:OE1	1:B:44:ILE:HD11	1.97	0.65
1:D:15:MET:HE2	1:D:18:ASN:ND2	2.12	0.65
1:A:42:GLN:OE1	1:A:44:ILE:HD11	1.97	0.64
1:B:110:VAL:O	1:B:114:ILE:HG13	1.97	0.64
1:B:306:LEU:C	1:B:307:ASN:O	2.40	0.64
1:C:306:LEU:C	1:C:307:ASN:O	2.40	0.64
1:A:15:MET:HE2	1:A:18:ASN:ND2	2.13	0.64
1:B:87:ARG:CG	1:B:88:ASP:N	2.51	0.64
1:B:15:MET:HE2	1:B:18:ASN:ND2	2.13	0.64
1:A:110:VAL:O	1:A:114:ILE:HG13	1.97	0.64
1:B:49:VAL:HG22	1:B:78:ILE:HD12	1.79	0.64
1:C:15:MET:HE2	1:C:18:ASN:ND2	2.13	0.64
1:A:49:VAL:HG22	1:A:78:ILE:HD12	1.79	0.64
1:A:192:GLU:HB2	1:A:321:LEU:HD11	1.80	0.64
1:C:110:VAL:O	1:C:114:ILE:HG13	1.97	0.64
1:D:42:GLN:OE1	1:D:44:ILE:HD11	1.97	0.64
1:C:42:GLN:OE1	1:C:44:ILE:HD11	1.97	0.64
1:B:192:GLU:HB2	1:B:321:LEU:HD11	1.80	0.64
1:C:192:GLU:HB2	1:C:321:LEU:HD11	1.80	0.64
1:B:18:ASN:N	1:B:18:ASN:ND2	2.24	0.63
1:C:49:VAL:HG22	1:C:78:ILE:HD12	1.79	0.63
1:D:49:VAL:HG22	1:D:78:ILE:HD12	1.79	0.63
1:D:257:ARG:HG3	1:D:257:ARG:HH11	1.61	0.63
1:A:265:ASN:ND2	1:A:295:ARG:CB	2.59	0.63
1:D:192:GLU:HB2	1:D:321:LEU:HD11	1.80	0.63
1:B:35:TYR:O	1:B:38:ALA:HB3	1.98	0.63
1:C:35:TYR:O	1:C:38:ALA:HB3	1.99	0.63
1:D:35:TYR:O	1:D:38:ALA:HB3	1.98	0.63
1:A:83:TYR:C	1:A:85:ASP:N	2.57	0.63
1:D:83:TYR:C	1:D:85:ASP:N	2.57	0.63
1:C:83:TYR:C	1:C:85:ASP:N	2.57	0.63
1:A:35:TYR:O	1:A:38:ALA:HB3	1.98	0.62
1:A:70:VAL:HG22	1:C:182:PRO:CB	2.29	0.62
1:B:182:PRO:CB	1:D:70:VAL:HG22	2.29	0.62
1:A:182:PRO:CB	1:C:70:VAL:HG22	2.29	0.62
1:D:324:VAL:O	1:D:328:ALA:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:PHE:CZ	1:B:131:GLY:HA3	2.35	0.62
1:C:324:VAL:O	1:C:328:ALA:HB3	2.00	0.62
1:A:243:LYS:HD3	1:C:59:ILE:HG22	1.82	0.62
1:B:324:VAL:O	1:B:328:ALA:HB3	1.99	0.62
1:C:129:PHE:CZ	1:C:131:GLY:HA3	2.35	0.62
1:B:70:VAL:HG22	1:D:182:PRO:CB	2.29	0.62
1:D:132:LEU:HD12	1:D:262:ILE:HG21	1.82	0.61
1:A:132:LEU:HD12	1:A:262:ILE:HG21	1.82	0.61
1:A:324:VAL:O	1:A:328:ALA:HB3	1.99	0.61
1:D:28:ALA:HB2	1:D:50:LEU:CD1	2.30	0.61
1:B:265:ASN:ND2	1:B:295:ARG:CB	2.60	0.61
1:B:59:ILE:HG22	1:D:243:LYS:HD3	1.82	0.61
1:D:15:MET:HE1	1:D:18:ASN:HA	1.83	0.61
1:A:59:ILE:HG22	1:C:243:LYS:HD3	1.82	0.61
1:B:28:ALA:HB2	1:B:50:LEU:CD1	2.31	0.61
1:B:73:PRO:O	1:B:74:LYS:HB2	2.01	0.61
1:D:129:PHE:CZ	1:D:131:GLY:HA3	2.35	0.61
1:B:295:ARG:HG3	1:B:295:ARG:NH1	2.15	0.61
1:C:331:ARG:C	1:C:331:ARG:HD3	2.26	0.61
1:A:28:ALA:HB2	1:A:50:LEU:CD1	2.30	0.61
1:A:129:PHE:CZ	1:A:131:GLY:HA3	2.35	0.61
1:A:306:LEU:C	1:A:307:ASN:O	2.40	0.61
1:C:132:LEU:HD12	1:C:262:ILE:HG21	1.82	0.61
1:D:73:PRO:O	1:D:74:LYS:HB2	2.00	0.61
1:B:178:PHE:CD1	1:B:206:ILE:HD13	2.36	0.61
1:C:15:MET:HE1	1:C:18:ASN:HA	1.83	0.61
1:A:178:PHE:CD1	1:A:206:ILE:HD13	2.36	0.61
1:C:28:ALA:HB2	1:C:50:LEU:CD1	2.30	0.61
1:B:243:LYS:HD3	1:D:59:ILE:HG22	1.82	0.60
1:D:178:PHE:CD1	1:D:206:ILE:HD13	2.36	0.60
1:D:331:ARG:HD3	1:D:331:ARG:C	2.26	0.60
1:C:73:PRO:O	1:C:74:LYS:HB2	2.01	0.60
1:C:178:PHE:CD1	1:C:206:ILE:HD13	2.36	0.60
1:D:189:ILE:HD11	1:D:233:VAL:HG11	1.84	0.60
1:D:306:LEU:C	1:D:307:ASN:O	2.40	0.60
1:A:331:ARG:HD3	1:A:331:ARG:C	2.26	0.60
1:B:331:ARG:HD3	1:B:331:ARG:C	2.26	0.60
1:A:15:MET:HE1	1:A:18:ASN:HA	1.83	0.60
1:A:324:VAL:O	1:A:324:VAL:HG12	2.02	0.60
1:B:132:LEU:HD12	1:B:262:ILE:HG21	1.82	0.60
1:A:189:ILE:HD11	1:A:233:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:CG	1:D:88:ASP:N	2.52	0.60
1:A:73:PRO:O	1:A:74:LYS:HB2	2.01	0.59
1:C:190:ILE:HD13	1:C:200:VAL:HG21	1.83	0.59
1:D:190:ILE:HD13	1:D:200:VAL:HG21	1.83	0.59
1:A:87:ARG:HB2	1:A:87:ARG:HH11	1.66	0.59
1:B:15:MET:HE1	1:B:18:ASN:HA	1.83	0.59
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.83	0.59
1:D:192:GLU:O	1:D:197:GLU:HB3	2.02	0.59
1:B:189:ILE:HD11	1:B:233:VAL:HG11	1.83	0.59
1:C:272:VAL:O	1:C:288:GLY:HA2	2.03	0.59
1:A:190:ILE:HD13	1:A:200:VAL:HG21	1.83	0.59
1:B:190:ILE:HD13	1:B:200:VAL:HG21	1.83	0.59
1:C:142:ILE:HD13	1:C:324:VAL:CG1	2.20	0.59
1:B:83:TYR:C	1:B:85:ASP:N	2.57	0.59
1:B:324:VAL:O	1:B:324:VAL:HG12	2.02	0.59
1:C:324:VAL:O	1:C:324:VAL:CG1	2.51	0.59
1:A:324:VAL:CG1	1:A:324:VAL:O	2.51	0.59
1:C:87:ARG:HB2	1:C:87:ARG:HH11	1.65	0.59
1:D:324:VAL:O	1:D:324:VAL:CG1	2.51	0.59
1:B:324:VAL:O	1:B:324:VAL:CG1	2.51	0.59
1:C:192:GLU:O	1:C:197:GLU:HB3	2.03	0.58
1:D:55:GLU:HG3	1:D:59:ILE:CD1	2.33	0.58
1:A:55:GLU:HG3	1:A:59:ILE:CD1	2.33	0.58
1:A:192:GLU:O	1:A:197:GLU:HB3	2.02	0.58
1:B:272:VAL:O	1:B:288:GLY:HA2	2.03	0.58
1:C:15:MET:CG	1:C:16:LYS:H	2.17	0.58
1:B:55:GLU:HG3	1:B:59:ILE:CD1	2.33	0.58
1:B:189:ILE:HG23	1:B:197:GLU:HG3	1.86	0.58
1:C:55:GLU:HG3	1:C:59:ILE:CD1	2.33	0.58
1:A:189:ILE:HG23	1:A:197:GLU:HG3	1.86	0.58
1:A:249:TYR:O	1:A:250:GLY:C	2.47	0.58
1:A:272:VAL:O	1:A:288:GLY:HA2	2.03	0.58
1:C:15:MET:HG3	1:C:16:LYS:N	2.19	0.58
1:C:295:ARG:HG3	1:C:295:ARG:NH1	2.15	0.58
1:D:87:ARG:HB2	1:D:87:ARG:HH11	1.66	0.58
1:A:15:MET:CG	1:A:16:LYS:H	2.16	0.58
1:D:132:LEU:HD12	1:D:262:ILE:CG2	2.34	0.58
1:B:240:ILE:HG13	1:B:247:THR:HG22	1.86	0.58
1:C:249:TYR:O	1:C:250:GLY:C	2.47	0.58
1:D:324:VAL:O	1:D:324:VAL:HG12	2.02	0.58
1:A:15:MET:HG3	1:A:16:LYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HD12	1:C:262:ILE:CG2	2.34	0.58
1:B:87:ARG:HB2	1:B:87:ARG:HH11	1.66	0.57
1:B:192:GLU:O	1:B:197:GLU:HB3	2.03	0.57
1:D:272:VAL:O	1:D:288:GLY:HA2	2.03	0.57
1:A:32:GLY:O	1:A:36:VAL:HG23	2.05	0.57
1:B:15:MET:HG3	1:B:16:LYS:N	2.18	0.57
1:C:324:VAL:O	1:C:324:VAL:HG12	2.02	0.57
1:D:32:GLY:O	1:D:36:VAL:HG23	2.04	0.57
1:A:15:MET:CG	1:A:16:LYS:N	2.66	0.57
1:A:240:ILE:HG13	1:A:247:THR:HG22	1.86	0.57
1:C:189:ILE:HG23	1:C:197:GLU:HG3	1.86	0.57
1:A:307:ASN:C	1:A:309:ASP:H	2.12	0.57
1:B:249:TYR:O	1:B:250:GLY:C	2.47	0.57
1:B:307:ASN:C	1:B:309:ASP:H	2.12	0.57
1:B:132:LEU:HD12	1:B:262:ILE:CG2	2.34	0.57
1:C:240:ILE:HG13	1:C:247:THR:HG22	1.86	0.57
1:A:132:LEU:HD12	1:A:262:ILE:CG2	2.34	0.57
1:D:15:MET:HE2	1:D:18:ASN:HA	1.87	0.57
1:A:28:ALA:HB2	1:A:50:LEU:HD11	1.87	0.56
1:B:15:MET:CG	1:B:16:LYS:N	2.67	0.56
1:A:169:ARG:NH1	2:A:1:SO4:O2	2.35	0.56
1:A:279:LEU:HG	1:A:303:GLU:HG3	1.88	0.56
1:C:32:GLY:O	1:C:36:VAL:HG23	2.04	0.56
1:C:170:PHE:HB2	1:C:189:ILE:HD12	1.88	0.56
1:D:15:MET:CG	1:D:16:LYS:H	2.16	0.56
1:D:142:ILE:HD13	1:D:324:VAL:CG1	2.20	0.56
1:D:189:ILE:HG23	1:D:197:GLU:HG3	1.86	0.56
1:D:15:MET:HG3	1:D:16:LYS:N	2.18	0.56
1:D:279:LEU:HG	1:D:303:GLU:HG3	1.87	0.56
1:B:15:MET:CG	1:B:16:LYS:H	2.17	0.56
1:B:28:ALA:HB2	1:B:50:LEU:HD11	1.88	0.56
1:B:275:TYR:O	1:B:277:ASP:OD1	2.24	0.56
1:C:279:LEU:HG	1:C:303:GLU:HG3	1.88	0.56
1:D:170:PHE:HB2	1:D:189:ILE:HD12	1.87	0.56
1:D:240:ILE:HG13	1:D:247:THR:HG22	1.86	0.56
1:B:142:ILE:HD13	1:B:324:VAL:CG1	2.21	0.56
1:C:15:MET:HE2	1:C:18:ASN:HA	1.87	0.56
1:D:249:TYR:O	1:D:250:GLY:C	2.47	0.56
1:D:295:ARG:HG3	1:D:295:ARG:NH1	2.15	0.56
1:D:307:ASN:C	1:D:309:ASP:H	2.12	0.56
1:A:125:MET:HE3	1:A:129:PHE:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HD11	1:A:211:ILE:HD11	1.88	0.56
1:A:299:ARG:NH1	1:D:179:SER:O	2.36	0.56
1:B:179:SER:O	1:C:299:ARG:NH1	2.36	0.56
1:D:206:ILE:HD11	1:D:211:ILE:HD11	1.88	0.56
1:D:275:TYR:O	1:D:277:ASP:OD1	2.24	0.56
1:A:64:ASP:OD2	1:C:244:LYS:NZ	2.39	0.55
1:A:179:SER:O	1:D:299:ARG:NH1	2.36	0.55
1:A:244:LYS:NZ	1:C:64:ASP:OD2	2.39	0.55
1:C:307:ASN:C	1:C:309:ASP:H	2.12	0.55
1:D:125:MET:HE3	1:D:129:PHE:HD2	1.71	0.55
1:A:170:PHE:HB2	1:A:189:ILE:HD12	1.87	0.55
1:B:64:ASP:OD2	1:D:244:LYS:NZ	2.40	0.55
1:C:275:TYR:O	1:C:277:ASP:OD1	2.24	0.55
1:B:32:GLY:O	1:B:36:VAL:HG23	2.05	0.55
1:B:113:ASN:ND2	1:B:116:ILE:HD12	2.22	0.55
1:B:244:LYS:NZ	1:D:64:ASP:OD2	2.39	0.55
1:B:125:MET:HE3	1:B:129:PHE:HD2	1.71	0.55
1:B:15:MET:HE2	1:B:18:ASN:HA	1.87	0.55
1:D:28:ALA:HB2	1:D:50:LEU:HD11	1.87	0.55
1:D:113:ASN:ND2	1:D:116:ILE:HD12	2.22	0.55
1:A:15:MET:HE2	1:A:18:ASN:HA	1.87	0.55
1:B:112:LYS:CB	1:B:112:LYS:NZ	2.70	0.55
1:D:15:MET:CG	1:D:16:LYS:N	2.67	0.55
1:D:112:LYS:CB	1:D:112:LYS:NZ	2.70	0.55
1:B:206:ILE:HD11	1:B:211:ILE:HD11	1.89	0.55
1:B:279:LEU:HG	1:B:303:GLU:HG3	1.88	0.55
1:C:15:MET:CG	1:C:16:LYS:N	2.67	0.55
1:C:279:LEU:HD23	1:C:301:VAL:HG12	1.89	0.55
1:A:113:ASN:ND2	1:A:116:ILE:HD12	2.22	0.55
1:A:275:TYR:O	1:A:277:ASP:OD1	2.24	0.55
1:A:112:LYS:NZ	1:A:112:LYS:CB	2.70	0.55
1:C:266:GLU:HG2	1:D:74:LYS:HE2	1.89	0.55
1:D:279:LEU:HD23	1:D:301:VAL:HG12	1.89	0.55
1:C:113:ASN:ND2	1:C:116:ILE:HD12	2.22	0.54
1:D:15:MET:HE2	1:D:18:ASN:CA	2.37	0.54
1:B:170:PHE:HB2	1:B:189:ILE:HD12	1.88	0.54
1:C:15:MET:HE2	1:C:18:ASN:CA	2.37	0.54
1:C:28:ALA:HB2	1:C:50:LEU:HD11	1.88	0.54
1:B:15:MET:HE2	1:B:18:ASN:CA	2.37	0.54
1:C:125:MET:HE3	1:C:129:PHE:HD2	1.71	0.54
1:C:74:LYS:HE2	1:D:266:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ILE:HD11	1:D:211:ILE:CD1	2.38	0.54
1:D:229:ILE:O	1:D:233:VAL:HG23	2.08	0.54
1:A:266:GLU:HG2	1:B:74:LYS:HE2	1.89	0.54
1:C:112:LYS:NZ	1:C:112:LYS:CB	2.70	0.54
1:C:206:ILE:HD11	1:C:211:ILE:HD11	1.89	0.54
1:A:15:MET:HE2	1:A:18:ASN:CA	2.37	0.54
1:A:229:ILE:O	1:A:233:VAL:HG23	2.08	0.54
1:A:253:MET:CE	1:C:72:ALA:HB2	2.38	0.54
1:C:229:ILE:O	1:C:233:VAL:HG23	2.08	0.54
1:A:22:ARG:NH2	1:A:47:GLU:OE1	2.36	0.54
1:A:279:LEU:HD23	1:A:301:VAL:HG12	1.89	0.54
1:C:189:ILE:HD13	1:C:233:VAL:HG11	1.90	0.54
1:A:206:ILE:HD11	1:A:211:ILE:CD1	2.38	0.54
1:B:206:ILE:HD11	1:B:211:ILE:CD1	2.38	0.54
1:A:87:ARG:CG	1:A:88:ASP:N	2.51	0.53
1:B:86:CYS:HA	1:B:89:ALA:HB2	1.90	0.53
1:B:229:ILE:O	1:B:233:VAL:HG23	2.08	0.53
1:A:26:ILE:HD12	1:A:92:VAL:CG1	2.39	0.53
1:A:178:PHE:CD1	1:A:206:ILE:CD1	2.92	0.53
1:A:74:LYS:HE2	1:B:266:GLU:HG2	1.89	0.53
1:A:189:ILE:HD13	1:A:233:VAL:HG11	1.91	0.53
1:B:279:LEU:HD23	1:B:301:VAL:HG12	1.89	0.53
1:C:206:ILE:HD11	1:C:211:ILE:CD1	2.38	0.53
1:B:299:ARG:NH1	1:C:179:SER:O	2.36	0.53
1:C:167:THR:CG2	1:C:189:ILE:H	2.22	0.53
1:D:26:ILE:HD12	1:D:92:VAL:CG1	2.39	0.53
1:D:86:CYS:HA	1:D:89:ALA:HB2	1.90	0.53
1:B:26:ILE:HD12	1:B:92:VAL:CG1	2.38	0.53
1:A:113:ASN:HB3	1:A:143:LEU:HD21	1.90	0.53
1:B:167:THR:CG2	1:B:189:ILE:H	2.22	0.53
1:C:178:PHE:CD1	1:C:206:ILE:CD1	2.92	0.53
1:D:178:PHE:CD1	1:D:206:ILE:CD1	2.92	0.53
1:D:189:ILE:HD13	1:D:233:VAL:HG11	1.91	0.53
1:A:72:ALA:HB2	1:C:253:MET:CE	2.38	0.53
1:A:86:CYS:HA	1:A:89:ALA:HB2	1.90	0.53
1:B:72:ALA:HB2	1:D:253:MET:CE	2.38	0.53
1:D:113:ASN:HB3	1:D:143:LEU:HD21	1.91	0.53
1:B:253:MET:CE	1:D:72:ALA:HB2	2.38	0.52
1:C:113:ASN:HB3	1:C:143:LEU:HD21	1.90	0.52
1:C:283:ARG:H	1:C:322:LYS:HZ2	1.57	0.52
1:D:15:MET:CE	1:D:18:ASN:CA	2.86	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:NH2	1:D:47:GLU:OE1	2.36	0.52
1:B:93:VAL:HG22	1:B:134:LEU:HD23	1.91	0.52
1:B:113:ASN:HB3	1:B:143:LEU:HD21	1.90	0.52
1:B:178:PHE:CD1	1:B:206:ILE:CD1	2.91	0.52
1:C:15:MET:HG2	1:D:296:ASN:OD1	2.10	0.52
1:D:167:THR:CG2	1:D:189:ILE:H	2.22	0.52
1:A:15:MET:HG2	1:B:296:ASN:OD1	2.09	0.52
1:A:167:THR:CG2	1:A:189:ILE:H	2.22	0.52
1:B:189:ILE:HD13	1:B:233:VAL:HG11	1.90	0.52
1:B:15:MET:CE	1:B:18:ASN:CA	2.86	0.52
1:C:93:VAL:HG22	1:C:134:LEU:HD23	1.92	0.52
1:C:296:ASN:OD1	1:D:15:MET:HG2	2.09	0.52
1:C:26:ILE:HD12	1:C:92:VAL:CG1	2.39	0.52
1:A:200:VAL:HG11	1:A:304:ILE:HD11	1.92	0.52
1:C:15:MET:CE	1:C:18:ASN:CA	2.86	0.52
1:A:93:VAL:HG22	1:A:134:LEU:HD23	1.91	0.52
1:C:28:ALA:CB	1:C:50:LEU:HD11	2.40	0.52
1:C:86:CYS:HA	1:C:89:ALA:HB2	1.90	0.52
1:D:26:ILE:HG21	1:D:120:ILE:HD13	1.92	0.52
1:B:28:ALA:CB	1:B:50:LEU:HD11	2.40	0.51
1:D:93:VAL:HG22	1:D:134:LEU:HD23	1.91	0.51
1:C:26:ILE:HG21	1:C:120:ILE:HD13	1.92	0.51
1:A:15:MET:CE	1:A:18:ASN:N	2.74	0.51
1:A:296:ASN:OD1	1:B:15:MET:HG2	2.09	0.51
1:A:26:ILE:HD12	1:A:92:VAL:HG13	1.93	0.51
1:B:26:ILE:HG21	1:B:120:ILE:HD13	1.92	0.51
1:D:15:MET:CE	1:D:18:ASN:N	2.74	0.51
1:B:200:VAL:HG11	1:B:304:ILE:HD11	1.92	0.51
1:C:15:MET:CE	1:C:18:ASN:N	2.74	0.51
1:A:28:ALA:CB	1:A:50:LEU:HD11	2.40	0.51
1:C:267:ASN:ND2	1:C:299:ARG:CZ	2.74	0.51
1:D:28:ALA:CB	1:D:50:LEU:HD11	2.40	0.51
1:A:267:ASN:ND2	1:A:294:ASN:OD1	2.44	0.51
1:A:267:ASN:ND2	1:A:299:ARG:CZ	2.74	0.51
1:B:267:ASN:ND2	1:B:294:ASN:OD1	2.44	0.51
1:B:26:ILE:HD12	1:B:92:VAL:HG13	1.93	0.50
1:B:321:LEU:C	1:B:323:SER:H	2.19	0.50
1:B:22:ARG:NH2	1:B:47:GLU:OE1	2.37	0.50
1:A:15:MET:CE	1:A:18:ASN:CA	2.86	0.50
1:A:26:ILE:HG21	1:A:120:ILE:HD13	1.92	0.50
1:B:267:ASN:ND2	1:B:299:ARG:CZ	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ILE:HD12	1:D:92:VAL:HG13	1.93	0.50
1:D:125:MET:O	1:D:128:GLY:N	2.45	0.50
1:D:267:ASN:ND2	1:D:294:ASN:OD1	2.44	0.50
1:D:267:ASN:ND2	1:D:299:ARG:CZ	2.74	0.50
1:A:283:ARG:H	1:A:322:LYS:HZ2	1.58	0.50
1:B:15:MET:CE	1:B:18:ASN:N	2.74	0.50
1:A:280:TYR:HB2	1:A:314:PHE:CE2	2.47	0.50
1:C:18:ASN:N	1:C:18:ASN:ND2	2.24	0.50
1:B:280:TYR:HB2	1:B:314:PHE:CE2	2.47	0.50
1:C:267:ASN:ND2	1:C:294:ASN:OD1	2.45	0.49
1:A:270:LEU:CD1	1:A:293:ILE:HD12	2.40	0.49
1:D:200:VAL:HG11	1:D:304:ILE:HD11	1.92	0.49
1:D:321:LEU:C	1:D:323:SER:H	2.19	0.49
1:A:125:MET:O	1:A:128:GLY:N	2.45	0.49
1:C:55:GLU:C	1:C:59:ILE:HD12	2.37	0.49
1:D:283:ARG:H	1:D:322:LYS:HZ2	1.59	0.49
1:C:26:ILE:HD12	1:C:92:VAL:HG13	1.93	0.49
1:C:280:TYR:HB2	1:C:314:PHE:CE2	2.47	0.49
1:A:279:LEU:CD2	1:A:301:VAL:HB	2.43	0.49
1:B:279:LEU:CD2	1:B:301:VAL:HB	2.43	0.49
1:D:280:TYR:HB2	1:D:314:PHE:CE2	2.47	0.49
1:C:321:LEU:C	1:C:323:SER:H	2.19	0.48
1:C:279:LEU:CD2	1:C:301:VAL:HB	2.43	0.48
1:D:55:GLU:C	1:D:59:ILE:HD12	2.37	0.48
1:B:283:ARG:H	1:B:322:LYS:HZ2	1.59	0.48
1:D:170:PHE:HB2	1:D:189:ILE:CD1	2.43	0.48
1:A:26:ILE:CG2	1:A:120:ILE:HD13	2.44	0.48
1:B:55:GLU:C	1:B:59:ILE:HD12	2.38	0.48
1:D:279:LEU:CD2	1:D:301:VAL:HB	2.43	0.48
1:C:170:PHE:HB2	1:C:189:ILE:CD1	2.43	0.48
1:B:125:MET:O	1:B:128:GLY:N	2.45	0.48
1:D:26:ILE:CG2	1:D:120:ILE:HD13	2.43	0.48
1:D:112:LYS:O	1:D:116:ILE:HG13	2.14	0.48
1:D:164:ILE:HG21	1:D:164:ILE:HD13	1.53	0.48
1:A:55:GLU:C	1:A:59:ILE:HD12	2.38	0.48
1:A:279:LEU:C	1:A:281:GLY:H	2.22	0.48
1:C:279:LEU:C	1:C:281:GLY:H	2.22	0.48
1:D:206:ILE:CD1	1:D:211:ILE:HD11	2.44	0.47
1:B:26:ILE:CG2	1:B:120:ILE:HD13	2.44	0.47
1:A:324:VAL:O	1:A:328:ALA:CB	2.62	0.47
1:B:170:PHE:HB2	1:B:189:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:O	1:C:116:ILE:HG13	2.14	0.47
1:A:170:PHE:HB2	1:A:189:ILE:CD1	2.43	0.47
1:B:59:ILE:HG13	1:B:79:TRP:CD1	2.50	0.47
1:B:112:LYS:O	1:B:116:ILE:HG13	2.14	0.47
1:A:206:ILE:CD1	1:A:211:ILE:HD11	2.44	0.47
1:C:125:MET:O	1:C:128:GLY:N	2.45	0.47
1:C:321:LEU:C	1:C:323:SER:N	2.72	0.47
1:C:324:VAL:O	1:C:328:ALA:CB	2.62	0.47
1:D:270:LEU:CD1	1:D:293:ILE:HD12	2.40	0.47
1:A:112:LYS:O	1:A:116:ILE:HG13	2.14	0.47
1:A:209:MET:HE1	1:D:305:GLU:HB3	1.97	0.47
1:A:321:LEU:C	1:A:323:SER:N	2.72	0.47
1:B:42:GLN:OE1	1:B:44:ILE:CD1	2.63	0.47
1:C:26:ILE:CG2	1:C:120:ILE:HD13	2.43	0.47
1:C:59:ILE:HG13	1:C:79:TRP:CD1	2.50	0.47
1:C:87:ARG:CG	1:C:88:ASP:N	2.51	0.47
1:C:302:ILE:HG21	1:C:302:ILE:HD13	1.60	0.47
1:A:42:GLN:OE1	1:A:44:ILE:CD1	2.63	0.47
1:A:59:ILE:HG13	1:A:79:TRP:CD1	2.50	0.47
1:B:22:ARG:O	1:B:90:ASP:HB2	2.15	0.47
1:B:96:ALA:O	1:B:137:THR:HG21	2.15	0.47
1:C:206:ILE:CD1	1:C:211:ILE:HD11	2.44	0.47
1:A:305:GLU:HB3	1:D:209:MET:HE1	1.97	0.47
1:D:24:VAL:HA	1:D:49:VAL:O	2.15	0.47
1:D:228:ARG:HD2	1:D:228:ARG:HA	1.56	0.47
1:A:228:ARG:HD2	1:A:228:ARG:HA	1.55	0.47
1:B:270:LEU:CD1	1:B:293:ILE:HD12	2.40	0.47
1:C:200:VAL:HG11	1:C:304:ILE:HD11	1.92	0.47
1:D:96:ALA:O	1:D:137:THR:HG21	2.15	0.47
1:D:324:VAL:O	1:D:328:ALA:CB	2.62	0.47
1:A:160:GLY:HA3	1:A:273:SER:HB2	1.97	0.46
1:B:206:ILE:CD1	1:B:211:ILE:HD11	2.44	0.46
1:C:129:PHE:CZ	1:C:131:GLY:CA	2.98	0.46
1:D:160:GLY:HA3	1:D:273:SER:HB2	1.97	0.46
1:A:321:LEU:C	1:A:323:SER:H	2.19	0.46
1:B:279:LEU:C	1:B:281:GLY:H	2.22	0.46
1:C:160:GLY:HA3	1:C:273:SER:HB2	1.97	0.46
1:D:129:PHE:CZ	1:D:131:GLY:CA	2.99	0.46
1:D:279:LEU:C	1:D:281:GLY:H	2.22	0.46
1:A:24:VAL:HA	1:A:49:VAL:O	2.15	0.46
1:B:293:ILE:O	1:B:294:ASN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:HA	1:C:49:VAL:O	2.15	0.46
1:C:138:ASN:HA	1:C:140:VAL:N	2.31	0.46
1:D:22:ARG:O	1:D:90:ASP:HB2	2.15	0.46
1:A:96:ALA:O	1:A:137:THR:HG21	2.15	0.46
1:A:295:ARG:HG3	1:A:295:ARG:NH1	2.15	0.46
1:B:164:ILE:HD13	1:B:164:ILE:HG21	1.52	0.46
1:C:96:ALA:O	1:C:137:THR:HG21	2.15	0.46
1:B:129:PHE:CZ	1:B:131:GLY:CA	2.98	0.46
1:D:167:THR:HG22	1:D:189:ILE:HB	1.98	0.46
1:A:22:ARG:O	1:A:90:ASP:HB2	2.15	0.46
1:D:59:ILE:HG13	1:D:79:TRP:CD1	2.50	0.46
1:B:24:VAL:HA	1:B:49:VAL:O	2.15	0.46
1:B:160:GLY:HA3	1:B:273:SER:HB2	1.97	0.46
1:B:324:VAL:O	1:B:328:ALA:CB	2.62	0.46
1:D:138:ASN:HA	1:D:140:VAL:N	2.31	0.46
1:B:240:ILE:CD1	1:B:247:THR:HG22	2.45	0.46
1:B:321:LEU:C	1:B:323:SER:N	2.73	0.46
1:C:167:THR:HG22	1:C:189:ILE:HB	1.98	0.46
1:D:293:ILE:O	1:D:294:ASN:HB3	2.15	0.46
1:A:253:MET:HE2	1:C:40:MET:HE2	1.98	0.46
1:B:118:ARG:CZ	1:B:122:GLU:OE2	2.64	0.46
1:A:234:ARG:O	1:A:234:ARG:HG2	2.17	0.45
1:B:138:ASN:HA	1:B:140:VAL:N	2.31	0.45
1:B:253:MET:HE2	1:D:40:MET:HE2	1.98	0.45
1:C:22:ARG:NH2	1:C:47:GLU:OE1	2.37	0.45
1:D:118:ARG:CZ	1:D:122:GLU:OE2	2.64	0.45
1:D:321:LEU:C	1:D:323:SER:N	2.72	0.45
1:D:328:ALA:O	1:D:329:PHE:CB	2.59	0.45
1:A:138:ASN:HA	1:A:140:VAL:N	2.31	0.45
1:A:240:ILE:CD1	1:A:247:THR:HG22	2.45	0.45
1:B:209:MET:HE1	1:C:305:GLU:HB3	1.97	0.45
1:B:240:ILE:HG12	1:B:247:THR:HG22	1.97	0.45
1:C:22:ARG:O	1:C:90:ASP:HB2	2.15	0.45
1:C:42:GLN:OE1	1:C:44:ILE:CD1	2.63	0.45
1:C:164:ILE:HG21	1:C:164:ILE:HD13	1.52	0.45
1:D:149:LYS:HA	1:D:149:LYS:HD3	1.73	0.45
1:D:240:ILE:CD1	1:D:247:THR:HG22	2.45	0.45
1:A:129:PHE:CZ	1:A:131:GLY:CA	2.98	0.45
1:A:167:THR:HG22	1:A:189:ILE:HB	1.98	0.45
1:B:243:LYS:HD3	1:D:59:ILE:CG2	2.45	0.45
1:C:118:ARG:CZ	1:C:122:GLU:OE2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2:SO4:O2	1:D:186:HIS:NE2	2.42	0.45
1:B:167:THR:HG22	1:B:189:ILE:HB	1.98	0.45
1:B:305:GLU:HB3	1:C:209:MET:HE1	1.97	0.45
1:C:209:MET:C	1:C:210:PRO:O	2.59	0.45
1:C:293:ILE:O	1:C:294:ASN:HB3	2.15	0.45
1:A:258:VAL:HG13	1:A:293:ILE:HD13	1.98	0.45
1:A:293:ILE:O	1:A:294:ASN:HB3	2.15	0.45
1:B:40:MET:HE2	1:D:253:MET:HE2	1.98	0.45
1:C:232:ASN:HD22	1:C:232:ASN:HA	1.40	0.45
1:A:232:ASN:HD22	1:A:232:ASN:HA	1.41	0.45
1:C:112:LYS:HZ3	1:C:112:LYS:HB3	1.82	0.45
1:C:240:ILE:CD1	1:C:247:THR:HG22	2.46	0.45
1:D:112:LYS:HB3	1:D:112:LYS:HZ3	1.80	0.45
1:B:72:ALA:HB2	1:D:253:MET:HE1	1.99	0.45
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.73	0.45
1:C:270:LEU:CD1	1:C:293:ILE:HD12	2.40	0.45
1:D:240:ILE:HD11	1:D:247:THR:HG22	1.99	0.45
1:A:40:MET:HE2	1:C:253:MET:HE2	1.98	0.45
1:A:260:ARG:HH11	1:A:260:ARG:HD3	1.04	0.45
1:C:234:ARG:O	1:C:234:ARG:HG2	2.17	0.45
1:A:118:ARG:CZ	1:A:122:GLU:OE2	2.64	0.45
1:A:304:ILE:HG21	1:A:304:ILE:HD13	1.74	0.45
1:B:258:VAL:HG13	1:B:293:ILE:HD13	1.98	0.45
1:D:42:GLN:OE1	1:D:44:ILE:CD1	2.63	0.45
1:A:59:ILE:CG2	1:C:243:LYS:HD3	2.45	0.44
1:A:243:LYS:HD3	1:C:59:ILE:CG2	2.45	0.44
1:C:136:ALA:HB2	1:C:255:LEU:HD21	1.99	0.44
1:B:161:SER:OG	1:B:251:ILE:HD11	2.17	0.44
1:D:113:ASN:C	1:D:115:ALA:N	2.76	0.44
1:B:59:ILE:CG2	1:D:243:LYS:HD3	2.45	0.44
1:C:240:ILE:HD11	1:C:247:THR:HG22	2.00	0.44
1:B:228:ARG:HA	1:B:228:ARG:HD2	1.55	0.44
1:B:260:ARG:HH11	1:B:260:ARG:HD3	1.04	0.44
1:D:258:VAL:HG13	1:D:293:ILE:HD13	1.99	0.44
1:A:48:ILE:HD13	1:A:48:ILE:HG21	1.74	0.44
1:A:136:ALA:HB2	1:A:255:LEU:HD21	1.99	0.44
1:B:327:ARG:HH11	1:B:327:ARG:HD3	1.59	0.44
1:C:161:SER:OG	1:C:251:ILE:HD11	2.18	0.44
1:A:161:SER:OG	1:A:251:ILE:HD11	2.18	0.44
1:A:164:ILE:HG21	1:A:164:ILE:HD13	1.53	0.44
1:C:258:VAL:HG13	1:C:293:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:HB3	1:B:112:LYS:HZ3	1.82	0.44
1:B:229:ILE:O	1:B:229:ILE:HG22	2.18	0.44
1:B:328:ALA:O	1:B:329:PHE:CB	2.59	0.44
1:D:161:SER:OG	1:D:251:ILE:HD11	2.18	0.44
1:D:322:LYS:HA	1:D:325:LEU:HD12	2.00	0.44
1:A:243:LYS:HE3	1:A:243:LYS:HB3	1.88	0.44
1:B:190:ILE:HD13	1:B:200:VAL:CG2	2.48	0.44
1:A:184:ASN:HB3	1:D:269:ILE:HD12	2.00	0.43
1:B:304:ILE:HD13	1:B:304:ILE:HG21	1.74	0.43
1:D:229:ILE:O	1:D:229:ILE:HG22	2.17	0.43
1:A:112:LYS:HZ3	1:A:112:LYS:HB3	1.83	0.43
1:A:322:LYS:HA	1:A:325:LEU:HD12	2.00	0.43
1:C:244:LYS:HE2	1:C:248:TYR:CZ	2.54	0.43
1:A:161:SER:CB	3:A:332:HOH:O	2.67	0.43
1:A:244:LYS:HE2	1:A:248:TYR:CZ	2.53	0.43
1:C:113:ASN:C	1:C:115:ALA:N	2.76	0.43
1:C:229:ILE:O	1:C:229:ILE:HG22	2.18	0.43
1:C:240:ILE:HG12	1:C:247:THR:HG22	1.98	0.43
1:D:136:ALA:HB2	1:D:255:LEU:HD21	1.99	0.43
1:D:167:THR:HG22	1:D:189:ILE:N	2.30	0.43
1:A:229:ILE:O	1:A:229:ILE:HG22	2.18	0.43
1:B:234:ARG:O	1:B:234:ARG:HG2	2.17	0.43
1:B:244:LYS:HE2	1:B:248:TYR:CZ	2.53	0.43
1:D:209:MET:C	1:D:210:PRO:O	2.59	0.43
1:B:253:MET:HE1	1:D:72:ALA:HB2	1.99	0.43
1:C:138:ASN:HA	1:C:140:VAL:H	1.84	0.43
1:A:240:ILE:HD11	1:A:247:THR:HG22	1.99	0.43
1:A:279:LEU:HD23	1:A:301:VAL:HG11	1.99	0.43
1:D:82:ASP:HB3	1:D:83:TYR:H	1.64	0.43
1:D:234:ARG:O	1:D:234:ARG:HG2	2.17	0.43
1:A:209:MET:C	1:A:210:PRO:O	2.59	0.43
1:B:136:ALA:HB2	1:B:255:LEU:HD21	2.00	0.43
1:C:167:THR:HG22	1:C:189:ILE:N	2.30	0.43
1:D:153:LEU:O	1:D:154:PRO:C	2.62	0.43
1:D:311:LYS:CA	1:D:315:HIS:CB	2.90	0.43
1:B:75:PRO:CD	1:B:75:PRO:O	2.67	0.43
1:B:126:ALA:C	1:B:128:GLY:H	2.27	0.43
1:B:232:ASN:HD22	1:B:232:ASN:HA	1.40	0.43
1:C:125:MET:HE3	1:C:129:PHE:CD2	2.54	0.43
1:D:138:ASN:HA	1:D:140:VAL:H	1.84	0.43
1:A:190:ILE:HD13	1:A:200:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:C	1:B:210:PRO:O	2.59	0.43
1:C:327:ARG:HH11	1:C:327:ARG:HD3	1.60	0.43
1:A:253:MET:HE1	1:C:72:ALA:HB2	1.99	0.43
1:A:113:ASN:C	1:A:115:ALA:H	2.27	0.42
1:A:138:ASN:HA	1:A:140:VAL:H	1.84	0.42
1:A:327:ARG:HH11	1:A:327:ARG:HD3	1.59	0.42
1:B:304:ILE:HA	1:C:209:MET:SD	2.59	0.42
1:D:75:PRO:CD	1:D:75:PRO:O	2.67	0.42
1:D:126:ALA:C	1:D:128:GLY:H	2.27	0.42
1:A:72:ALA:HB2	1:C:253:MET:HE1	1.99	0.42
1:B:269:ILE:HD12	1:C:184:ASN:HB3	2.01	0.42
1:C:322:LYS:HA	1:C:325:LEU:HD12	2.00	0.42
1:A:75:PRO:CD	1:A:75:PRO:O	2.67	0.42
1:A:304:ILE:HA	1:D:209:MET:SD	2.59	0.42
1:B:184:ASN:HB3	1:C:269:ILE:HD12	2.01	0.42
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.78	0.42
1:B:322:LYS:HA	1:B:325:LEU:HD12	2.00	0.42
1:B:15:MET:HE2	1:B:18:ASN:CG	2.44	0.42
1:B:279:LEU:HD23	1:B:301:VAL:HG11	1.99	0.42
1:D:302:ILE:HD13	1:D:302:ILE:HG21	1.60	0.42
1:A:125:MET:HE3	1:A:129:PHE:HB3	2.02	0.42
1:A:126:ALA:C	1:A:128:GLY:H	2.27	0.42
1:B:125:MET:HE3	1:B:129:PHE:HB3	2.02	0.42
1:B:138:ASN:HA	1:B:140:VAL:H	1.83	0.42
1:B:240:ILE:HD11	1:B:247:THR:HG22	1.99	0.42
1:D:15:MET:HE2	1:D:18:ASN:CG	2.44	0.42
1:D:244:LYS:HE2	1:D:248:TYR:CZ	2.53	0.42
1:A:167:THR:O	1:A:171:ARG:HG3	2.20	0.42
1:C:75:PRO:O	1:C:75:PRO:CD	2.67	0.42
1:C:293:ILE:HD13	1:C:293:ILE:HG21	1.83	0.42
1:B:165:LEU:O	1:B:169:ARG:HG3	2.20	0.42
1:C:279:LEU:HD23	1:C:301:VAL:HG11	1.99	0.42
1:D:113:ASN:C	1:D:115:ALA:H	2.27	0.42
1:D:190:ILE:HD13	1:D:200:VAL:CG2	2.48	0.42
1:A:132:LEU:CD1	1:A:262:ILE:CG2	2.98	0.42
1:C:132:LEU:CD1	1:C:262:ILE:CG2	2.98	0.42
1:A:136:ALA:HA	1:A:161:SER:HB2	2.02	0.42
1:A:165:LEU:O	1:A:169:ARG:HG3	2.20	0.42
1:A:269:ILE:HD12	1:D:184:ASN:HB3	2.01	0.42
1:A:280:TYR:CE2	1:A:289:VAL:CG2	3.03	0.42
1:B:209:MET:SD	1:C:304:ILE:HA	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ASN:C	1:C:115:ALA:H	2.27	0.42
1:C:126:ALA:C	1:C:128:GLY:H	2.27	0.42
1:D:167:THR:O	1:D:171:ARG:HG3	2.20	0.42
1:B:167:THR:O	1:B:171:ARG:HG3	2.20	0.42
1:C:149:LYS:HD3	1:C:149:LYS:HA	1.73	0.42
1:C:165:LEU:O	1:C:169:ARG:HG3	2.20	0.42
1:D:165:LEU:O	1:D:169:ARG:HG3	2.20	0.42
1:D:181:ALA:HA	1:D:182:PRO:HD3	1.82	0.42
1:D:279:LEU:HD23	1:D:301:VAL:HG11	1.99	0.42
1:C:181:ALA:HA	1:C:182:PRO:HD3	1.82	0.41
1:C:206:ILE:CD1	1:C:211:ILE:CD1	2.98	0.41
1:C:15:MET:HE2	1:C:18:ASN:CG	2.44	0.41
1:C:311:LYS:CA	1:C:315:HIS:CB	2.90	0.41
1:B:113:ASN:C	1:B:115:ALA:H	2.27	0.41
1:B:113:ASN:C	1:B:115:ALA:N	2.76	0.41
1:B:280:TYR:CE2	1:B:289:VAL:CG2	3.03	0.41
1:D:132:LEU:CD1	1:D:262:ILE:CG2	2.98	0.41
1:A:15:MET:HE2	1:A:18:ASN:CG	2.44	0.41
1:A:209:MET:SD	1:D:304:ILE:HA	2.60	0.41
1:C:125:MET:HE3	1:C:129:PHE:HB3	2.02	0.41
1:D:112:LYS:CB	1:D:112:LYS:HZ3	2.33	0.41
1:D:280:TYR:CE2	1:D:289:VAL:CG2	3.04	0.41
1:B:71:PHE:CE1	1:D:168:ALA:HB2	2.56	0.41
1:C:280:TYR:CE2	1:C:289:VAL:CG2	3.03	0.41
1:C:287:ILE:HD13	1:C:287:ILE:HG21	1.85	0.41
1:C:328:ALA:O	1:C:329:PHE:CB	2.59	0.41
1:A:125:MET:HE3	1:A:129:PHE:CD2	2.53	0.41
1:B:132:LEU:CD1	1:B:262:ILE:CG2	2.98	0.41
1:C:167:THR:O	1:C:171:ARG:HG3	2.20	0.41
1:A:27:GLY:O	1:A:32:GLY:HA3	2.21	0.41
1:A:114:ILE:O	1:A:114:ILE:HG22	2.21	0.41
1:A:168:ALA:HB2	1:C:71:PHE:CE1	2.56	0.41
1:B:153:LEU:O	1:B:154:PRO:C	2.62	0.41
1:A:199:PRO:O	1:A:199:PRO:HG2	2.21	0.41
1:B:203:GLN:O	1:C:208:VAL:HB	2.21	0.41
1:C:120:ILE:HD13	1:C:120:ILE:HG21	1.80	0.41
1:C:136:ALA:HA	1:C:161:SER:HB2	2.03	0.41
1:C:243:LYS:HE3	1:C:243:LYS:HB3	1.89	0.41
1:C:304:ILE:HD13	1:C:304:ILE:HG21	1.74	0.41
1:A:153:LEU:O	1:A:154:PRO:C	2.62	0.41
1:B:112:LYS:CB	1:B:112:LYS:HZ3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.82	0.41
1:C:199:PRO:O	1:C:199:PRO:HG2	2.21	0.41
1:C:331:ARG:C	1:C:331:ARG:CD	2.93	0.41
1:D:136:ALA:HA	1:D:161:SER:HB2	2.02	0.41
1:A:113:ASN:C	1:A:115:ALA:N	2.76	0.40
1:B:114:ILE:O	1:B:114:ILE:HG22	2.21	0.40
1:B:136:ALA:HA	1:B:161:SER:HB2	2.02	0.40
1:B:149:LYS:HA	1:B:149:LYS:HD3	1.73	0.40
1:B:199:PRO:O	1:B:199:PRO:HG2	2.21	0.40
1:B:208:VAL:HB	1:C:203:GLN:O	2.21	0.40
1:C:27:GLY:O	1:C:32:GLY:HA3	2.21	0.40
1:C:118:ARG:NH2	1:C:122:GLU:OE2	2.54	0.40
1:C:228:ARG:HA	1:C:228:ARG:HD2	1.56	0.40
1:A:42:GLN:HB2	1:A:44:ILE:HD12	2.03	0.40
1:A:206:ILE:CD1	1:A:211:ILE:CD1	2.98	0.40
1:A:279:LEU:C	1:A:281:GLY:N	2.79	0.40
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.86	0.40
1:C:42:GLN:HB2	1:C:44:ILE:HD12	2.03	0.40
1:D:112:LYS:NZ	1:D:112:LYS:HB3	2.36	0.40
1:D:118:ARG:NH2	1:D:122:GLU:OE2	2.54	0.40
1:D:279:LEU:C	1:D:281:GLY:N	2.79	0.40
1:A:71:PHE:CE1	1:C:168:ALA:HB2	2.56	0.40
1:A:118:ARG:NH2	1:A:122:GLU:OE2	2.55	0.40
1:B:27:GLY:O	1:B:32:GLY:HA3	2.21	0.40
1:B:118:ARG:NH2	1:B:122:GLU:OE2	2.55	0.40
1:B:125:MET:HE3	1:B:129:PHE:CD2	2.54	0.40
1:B:251:ILE:O	1:B:254:GLY:N	2.55	0.40
1:C:112:LYS:NZ	1:C:112:LYS:HB3	2.36	0.40
1:D:48:ILE:HD13	1:D:48:ILE:HG21	1.74	0.40
1:D:206:ILE:CD1	1:D:211:ILE:CD1	2.98	0.40
1:D:313:ARG:HH11	1:D:313:ARG:HG2	1.87	0.40
1:D:327:ARG:HH11	1:D:327:ARG:HD3	1.59	0.40
1:A:70:VAL:O	1:A:70:VAL:CG1	2.70	0.40
1:A:167:THR:HG22	1:A:189:ILE:N	2.30	0.40
1:C:279:LEU:C	1:C:281:GLY:N	2.79	0.40
1:D:27:GLY:O	1:D:32:GLY:HA3	2.21	0.40
1:D:125:MET:HE3	1:D:129:PHE:HB3	2.02	0.40

All (57) 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:A:326:ALA:N	1:D:331:ARG:CB[6_665]	0.71	1.49
1:A:326:ALA:C	1:D:331:ARG:C[6_665]	0.78	1.42
1:A:325:LEU:C	1:D:331:ARG:CB[6_665]	0.88	1.32
1:C:316:HIS:CE1	1:D:316:HIS:CE1[6_655]	1.07	1.13
1:C:316:HIS:NE2	1:D:316:HIS:CE1[6_655]	1.09	1.11
1:A:326:ALA:N	1:D:331:ARG:CA[6_665]	1.12	1.08
1:A:326:ALA:CA	1:D:331:ARG:C[6_665]	1.23	0.97
1:A:323:SER:C	1:D:330:THR:CB[6_665]	1.24	0.96
1:C:316:HIS:NE2	1:D:316:HIS:NE2[6_655]	1.24	0.96
1:A:325:LEU:O	1:D:331:ARG:CG[6_665]	1.28	0.92
1:A:327:ARG:CB	1:D:330:THR:O[6_665]	1.32	0.88
1:C:235:ASP:OD2	1:D:235:ASP:OD2[6_655]	1.34	0.86
1:A:323:SER:O	1:D:330:THR:CA[6_665]	1.42	0.78
1:A:323:SER:O	1:D:330:THR:CB[6_665]	1.42	0.78
1:A:327:ARG:N	1:D:331:ARG:C[6_665]	1.42	0.78
1:C:316:HIS:CE1	1:D:316:HIS:NE2[6_655]	1.48	0.72
1:A:326:ALA:CA	1:D:331:ARG:CA[6_665]	1.54	0.66
1:A:325:LEU:O	1:D:331:ARG:CB[6_665]	1.55	0.65
1:A:326:ALA:C	1:D:331:ARG:CA[6_665]	1.57	0.63
1:A:327:ARG:CA	1:D:330:THR:O[6_665]	1.59	0.61
1:A:327:ARG:N	1:D:331:ARG:CA[6_665]	1.59	0.61
1:A:323:SER:O	1:D:330:THR:C[6_665]	1.60	0.60
1:A:326:ALA:CA	1:D:331:ARG:CB[6_665]	1.60	0.60
1:A:324:VAL:N	1:D:330:THR:CB[6_665]	1.67	0.53
1:A:323:SER:O	1:D:330:THR:OG1[6_665]	1.68	0.52
1:A:323:SER:O	1:D:331:ARG:N[6_665]	1.70	0.50
1:A:326:ALA:CB	1:D:331:ARG:O[6_665]	1.70	0.50
1:A:323:SER:CB	1:D:330:THR:OG1[6_665]	1.72	0.48
1:A:326:ALA:CA	1:D:331:ARG:CG[6_665]	1.85	0.35
1:C:316:HIS:CD2	1:D:316:HIS:NE2[6_655]	1.88	0.32
1:A:323:SER:C	1:D:330:THR:OG1[6_665]	1.89	0.31
1:A:326:ALA:N	1:D:331:ARG:N[6_665]	1.89	0.31
1:A:326:ALA:CA	1:D:331:ARG:CD[6_665]	1.90	0.30
1:A:325:LEU:C	1:D:331:ARG:CG[6_665]	1.91	0.29
1:A:323:SER:OG	1:D:330:THR:CG2[6_665]	1.93	0.27
1:A:323:SER:CA	1:D:330:THR:OG1[6_665]	1.93	0.27
1:A:326:ALA:O	1:D:331:ARG:C[6_665]	1.95	0.25
1:A:327:ARG:N	1:D:331:ARG:N[6_665]	1.95	0.25
1:A:326:ALA:CA	1:D:331:ARG:O[6_665]	1.97	0.23
1:C:316:HIS:NE2	1:D:316:HIS:ND1[6_655]	1.97	0.23
1:A:326:ALA:CB	1:D:331:ARG:C[6_665]	2.00	0.20
1:A:327:ARG:CB	1:D:330:THR:C[6_665]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:C	1:D:331:ARG:O[6_665]	2.02	0.18
1:A:327:ARG:N	1:D:330:THR:O[6_665]	2.02	0.18
1:C:327:ARG:NH1	1:D:312:ASN:CG[6_655]	2.05	0.15
1:A:327:ARG:N	1:D:330:THR:C[6_665]	2.07	0.13
1:A:325:LEU:C	1:D:331:ARG:CA[6_665]	2.11	0.09
1:C:316:HIS:ND1	1:D:316:HIS:NE2[6_655]	2.11	0.09
1:A:327:ARG:C	1:D:330:THR:O[6_665]	2.12	0.08
1:A:327:ARG:N	1:D:331:ARG:O[6_665]	2.13	0.07
1:A:323:SER:CA	1:D:330:THR:CB[6_665]	2.14	0.06
1:A:327:ARG:CB	1:D:329:PHE:O[6_665]	2.14	0.06
1:C:316:HIS:NE2	1:D:316:HIS:CD2[6_655]	2.14	0.06
1:A:326:ALA:N	1:D:331:ARG:CG[6_665]	2.16	0.04
1:C:228:ARG:NE	1:D:242:GLU:OE2[6_655]	2.17	0.03
1:A:323:SER:C	1:D:330:THR:CA[6_665]	2.18	0.02
1:A:326:ALA:CB	1:D:331:ARG:CD[6_665]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
1	B	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
1	C	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
1	D	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
All	All	1144/1268 (90%)	928 (81%)	152 (13%)	64 (6%)	1	4

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	98	ALA

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Mol	Chain	Res	Type
1	A	307	ASN
1	A	311	LYS
1	A	329	PHE
1	B	18	ASN
1	B	98	ALA
1	B	307	ASN
1	B	311	LYS
1	B	329	PHE
1	C	18	ASN
1	C	98	ALA
1	C	307	ASN
1	C	311	LYS
1	C	329	PHE
1	D	18	ASN
1	D	98	ALA
1	D	307	ASN
1	D	311	LYS
1	D	329	PHE
1	A	75	PRO
1	A	330	THR
1	B	75	PRO
1	B	330	THR
1	C	75	PRO
1	C	330	THR
1	D	75	PRO
1	D	330	THR
1	A	284	ASP
1	B	284	ASP
1	C	284	ASP
1	D	284	ASP
1	A	250	GLY
1	B	250	GLY
1	C	250	GLY
1	D	250	GLY
1	A	248	TYR
1	B	248	TYR
1	C	248	TYR
1	D	248	TYR
1	A	210	PRO
1	A	267	ASN
1	B	210	PRO
1	B	267	ASN

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Mol	Chain	Res	Type
1	C	210	PRO
1	C	267	ASN
1	D	210	PRO
1	D	267	ASN
1	A	74	LYS
1	B	74	LYS
1	C	74	LYS
1	D	74	LYS
1	A	73	PRO
1	B	73	PRO
1	C	73	PRO
1	D	73	PRO
1	A	180	VAL
1	B	180	VAL
1	C	180	VAL
1	D	180	VAL
1	A	139	PRO
1	B	139	PRO
1	C	139	PRO
1	D	139	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/255 (92%)	206 (87%)	30 (13%)	4	15
1	B	236/255 (92%)	206 (87%)	30 (13%)	4	15
1	C	236/255 (92%)	206 (87%)	30 (13%)	4	15
1	D	236/255 (92%)	206 (87%)	30 (13%)	4	15
All	All	944/1020 (92%)	824 (87%)	120 (13%)	4	15

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET

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Mol	Chain	Res	Type
1	A	18	ASN
1	A	77	ASP
1	A	87	ARG
1	A	99	ASN
1	A	112	LYS
1	A	113	ASN
1	A	119	SER
1	A	125	MET
1	A	134	LEU
1	A	179	SER
1	A	183	GLN
1	A	192	GLU
1	A	197	GLU
1	A	198	LEU
1	A	203	GLN
1	A	211	ILE
1	A	227	GLU
1	A	228	ARG
1	A	243	LYS
1	A	257	ARG
1	A	265	ASN
1	A	266	GLU
1	A	283	ARG
1	A	289	VAL
1	A	294	ASN
1	A	295	ARG
1	A	312	ASN
1	A	320	THR
1	A	324	VAL
1	B	15	MET
1	B	18	ASN
1	B	77	ASP
1	B	87	ARG
1	B	99	ASN
1	B	112	LYS
1	B	113	ASN
1	B	119	SER
1	B	125	MET
1	B	134	LEU
1	B	179	SER
1	B	183	GLN
1	B	192	GLU

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Mol	Chain	Res	Type
1	B	197	GLU
1	B	198	LEU
1	B	203	GLN
1	B	211	ILE
1	B	227	GLU
1	B	228	ARG
1	B	243	LYS
1	B	257	ARG
1	B	265	ASN
1	B	266	GLU
1	B	283	ARG
1	B	289	VAL
1	B	294	ASN
1	B	295	ARG
1	B	312	ASN
1	B	320	THR
1	B	324	VAL
1	C	15	MET
1	C	18	ASN
1	C	77	ASP
1	C	87	ARG
1	C	99	ASN
1	C	112	LYS
1	C	113	ASN
1	C	119	SER
1	C	125	MET
1	C	134	LEU
1	C	179	SER
1	C	183	GLN
1	C	192	GLU
1	C	197	GLU
1	C	198	LEU
1	C	203	GLN
1	C	211	ILE
1	C	227	GLU
1	C	228	ARG
1	C	243	LYS
1	C	257	ARG
1	C	265	ASN
1	C	266	GLU
1	C	283	ARG
1	C	289	VAL

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Mol	Chain	Res	Type
1	C	294	ASN
1	C	295	ARG
1	C	312	ASN
1	C	320	THR
1	C	324	VAL
1	D	15	MET
1	D	18	ASN
1	D	77	ASP
1	D	87	ARG
1	D	99	ASN
1	D	112	LYS
1	D	113	ASN
1	D	119	SER
1	D	125	MET
1	D	134	LEU
1	D	179	SER
1	D	183	GLN
1	D	192	GLU
1	D	197	GLU
1	D	198	LEU
1	D	203	GLN
1	D	211	ILE
1	D	227	GLU
1	D	228	ARG
1	D	243	LYS
1	D	257	ARG
1	D	265	ASN
1	D	266	GLU
1	D	283	ARG
1	D	289	VAL
1	D	294	ASN
1	D	295	ARG
1	D	312	ASN
1	D	320	THR
1	D	324	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	99	ASN
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	138	ASN
1	A	232	ASN
1	A	265	ASN
1	A	267	ASN
1	A	294	ASN
1	A	307	ASN
1	B	18	ASN
1	B	99	ASN
1	B	113	ASN
1	B	138	ASN
1	B	193	HIS
1	B	232	ASN
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	296	ASN
1	B	307	ASN
1	C	18	ASN
1	C	99	ASN
1	C	113	ASN
1	C	138	ASN
1	C	193	HIS
1	C	232	ASN
1	C	265	ASN
1	C	267	ASN
1	C	294	ASN
1	C	307	ASN
1	D	18	ASN
1	D	99	ASN
1	D	113	ASN
1	D	138	ASN
1	D	193	HIS
1	D	232	ASN
1	D	265	ASN
1	D	267	ASN
1	D	294	ASN
1	D	296	ASN
1	D	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	2	-	4,4,4	1.23	1 (25%)	6,6,6	1.03	1 (16%)
2	SO4	A	1	-	4,4,4	0.95	0	6,6,6	0.75	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	SO4	O2-S	2.12	1.57	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	SO4	O4-S-O1	2.12	120.65	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.