



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:45 PM EDT

PDB ID : 1DLU / pdb_00001dlu
Title : UNLIGANDED BIOSYNTHETIC THIOLASE FROM ZOOGLOEA
RAMIGERA
Authors : Modis, Y.; Wierenga, R.K.
Deposited on : 1999-12-12
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

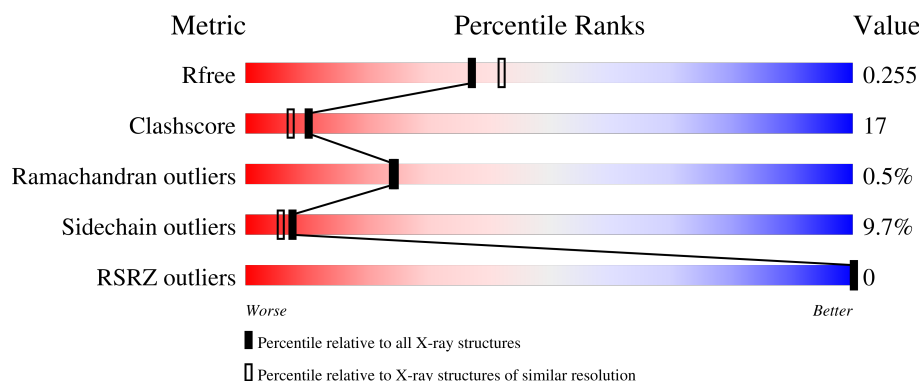
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

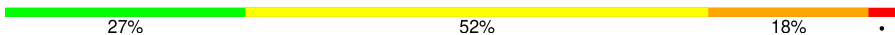
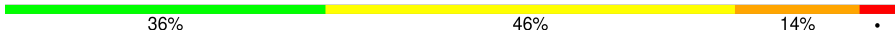
The reported resolution of this entry is 2.25 Å.

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))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	389	
1	B	389	
1	C	389	
1	D	389	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	A	1001	-	-	X	-
3	MPD	B	1002	-	-	X	-
3	MPD	C	1003	-	-	X	-
3	MPD	D	1004	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12065 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.

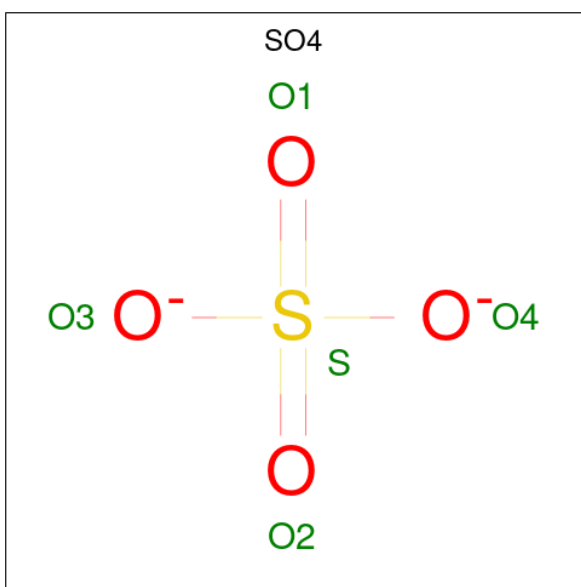
- Molecule 1 is a protein called BIOSYNTHETIC THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	B	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	C	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	D	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			

There are 8 discrepancies between the modelled and reference sequences:

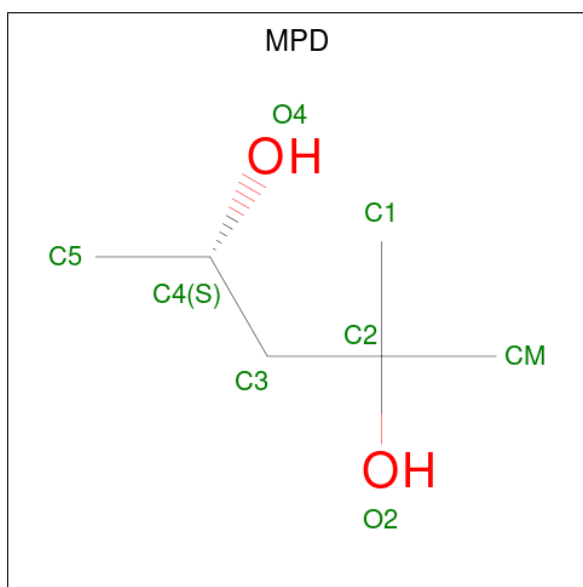
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	insertion	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	11	ALA	-	insertion	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	11	ALA	-	insertion	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	11	ALA	-	insertion	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- 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		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

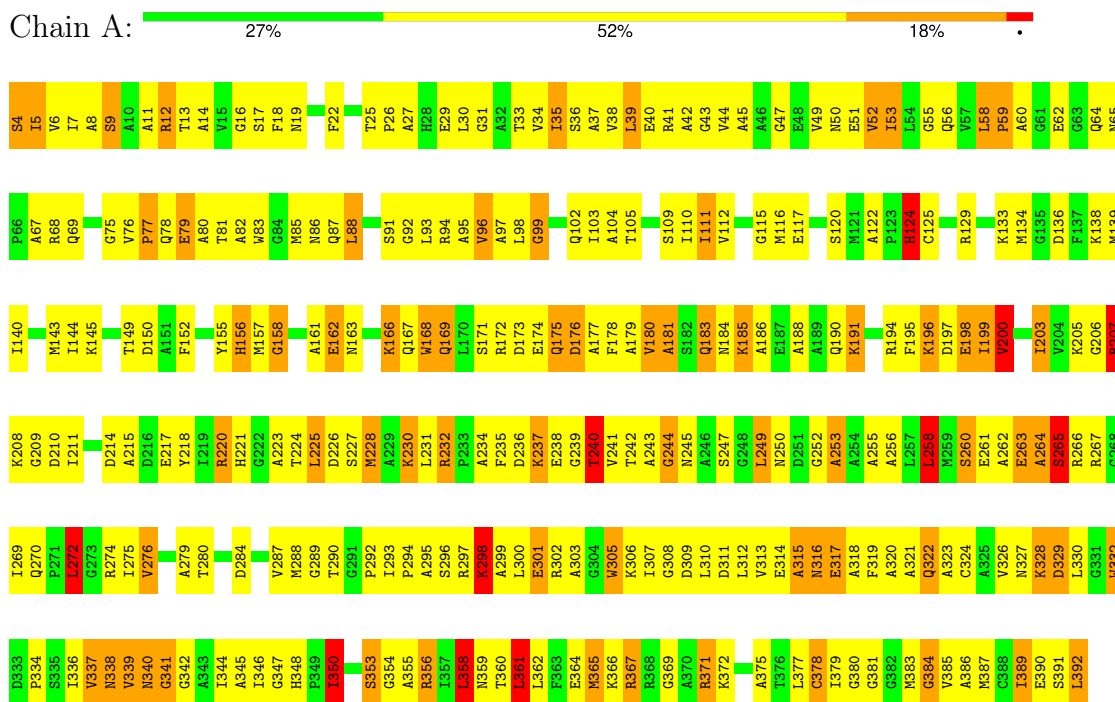
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	293	Total	O	4	0
			293	293		
4	B	287	Total	O	4	0
			287	287		
4	C	101	Total	O	3	0
			101	101		
4	D	70	Total	O	3	0
			70	70		

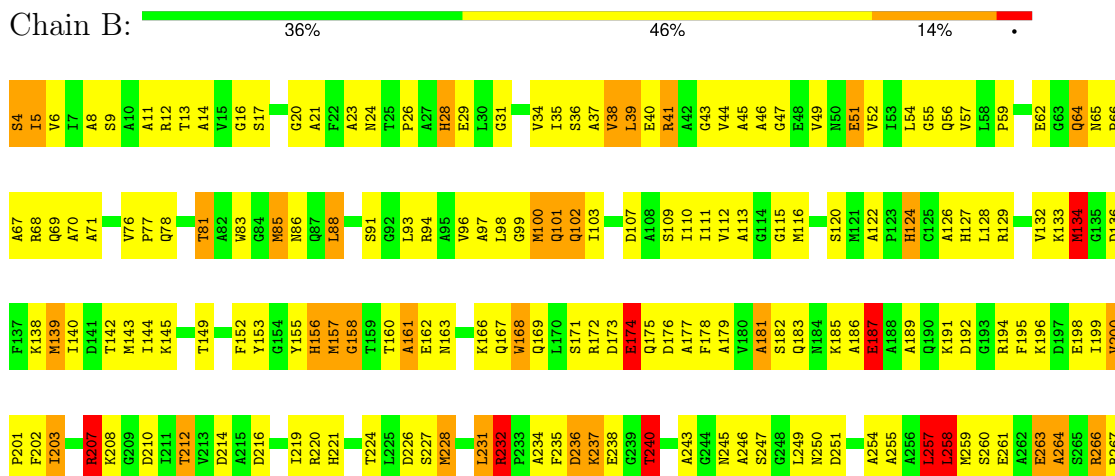
3 Residue-property plots

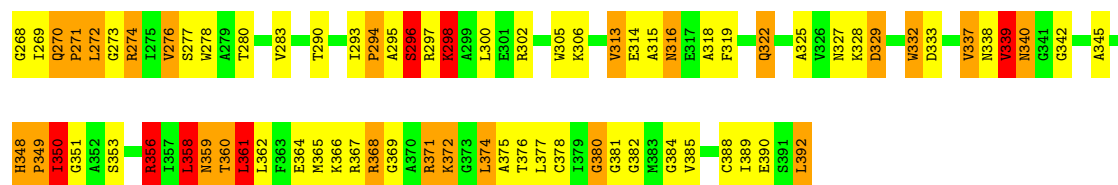
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: BIOSYNTHETIC THIOLASE



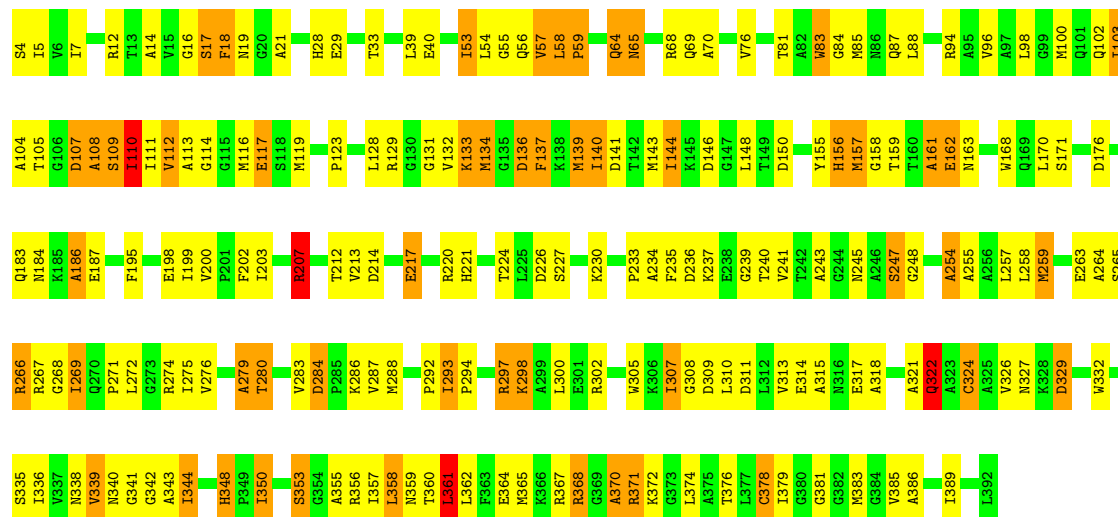
• Molecule 1: BIOSYNTHETIC THIOLASE





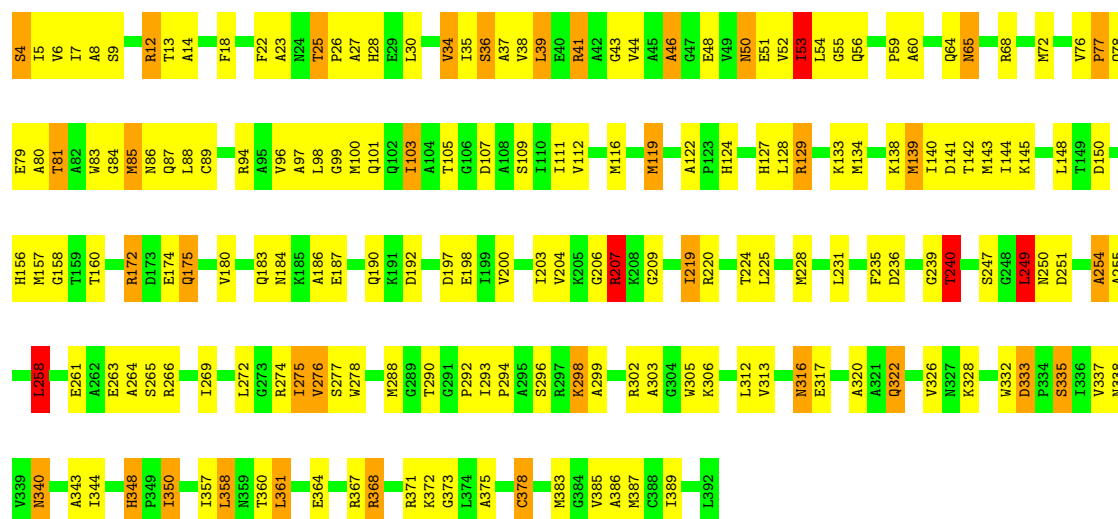
• Molecule 1: BIOSYNTHETIC THIOLASE

Chain C: 49% 37% 13%



• Molecule 1: BIOSYNTHETIC THIOLASE

Chain D: 53% 37% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.71Å 79.73Å 150.48Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.25) 84.1 (20.00-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.263 0.209 , 0.255	Depositor DCC
R_{free} test set	4898 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.985	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12065	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.68	24/2854 (0.8%)	3.34	467/3853 (12.1%)
1	B	1.59	23/2854 (0.8%)	3.06	384/3853 (10.0%)
1	C	0.80	0/2854	2.33	158/3853 (4.1%)
1	D	0.76	0/2854	2.21	114/3853 (3.0%)
All	All	1.28	47/11416 (0.4%)	2.78	1123/15412 (7.3%)

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	3
1	B	0	3
All	All	0	6

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	ARG	NE-CZ	-8.78	1.23	1.33
1	B	314	GLU	CA-CB	8.75	1.65	1.53
1	A	190	GLN	N-CA	-8.68	1.35	1.46
1	B	111	ILE	C-O	-8.42	1.15	1.24
1	B	88	LEU	C-O	7.27	1.33	1.24
1	A	179	ALA	N-CA	-7.12	1.38	1.46
1	B	179	ALA	C-N	7.07	1.42	1.34
1	B	337	VAL	C-N	6.91	1.43	1.33
1	A	324	CYS	N-CA	6.53	1.54	1.46
1	A	67	ALA	C-N	6.50	1.42	1.33
1	A	190	GLN	CA-CB	6.41	1.63	1.53
1	B	199	ILE	C-N	6.40	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	GLY	CA-C	6.29	1.59	1.52
1	A	272	LEU	N-CA	6.23	1.54	1.46
1	B	115	GLY	N-CA	6.14	1.51	1.45
1	B	201	PRO	N-CD	6.12	1.56	1.47
1	B	362	LEU	C-O	-6.12	1.17	1.24
1	A	199	ILE	N-CA	6.07	1.53	1.46
1	A	26	PRO	N-CA	-5.97	1.39	1.47
1	B	143	MET	N-CA	-5.93	1.39	1.46
1	A	97	ALA	N-CA	-5.92	1.39	1.46
1	B	55	GLY	CA-C	5.91	1.57	1.52
1	A	175	GLN	N-CA	-5.90	1.39	1.46
1	B	83	TRP	C-N	5.85	1.42	1.33
1	B	45	ALA	N-CA	5.85	1.52	1.45
1	B	17	SER	C-O	-5.79	1.16	1.23
1	A	27	ALA	C-O	-5.78	1.17	1.24
1	A	47	GLY	C-O	5.76	1.30	1.23
1	B	203	ILE	C-N	-5.73	1.28	1.33
1	A	112	VAL	N-CA	-5.71	1.39	1.46
1	B	45	ALA	C-N	5.61	1.41	1.34
1	A	315	ALA	C-N	-5.60	1.26	1.33
1	A	129	ARG	NE-CZ	-5.37	1.27	1.33
1	A	59	PRO	N-CD	5.31	1.55	1.47
1	B	172	ARG	NE-CZ	5.31	1.38	1.33
1	B	257	LEU	N-CA	5.27	1.52	1.46
1	A	99	GLY	CA-C	5.22	1.58	1.51
1	B	277	SER	C-O	-5.22	1.18	1.23
1	B	11	ALA	C-N	5.18	1.39	1.33
1	A	98	LEU	CA-CB	5.11	1.61	1.53
1	A	53	ILE	C-N	5.08	1.40	1.33
1	A	323	ALA	C-O	5.05	1.29	1.24
1	A	364	GLU	CA-C	5.03	1.59	1.52
1	A	95	ALA	N-CA	-5.03	1.40	1.46
1	B	59	PRO	N-CD	5.02	1.54	1.47
1	B	319	PHE	C-N	5.01	1.40	1.33
1	A	284	ASP	CA-C	-5.00	1.46	1.52

All (1123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	367	ARG	CD-NE-CZ	27.82	163.35	124.40
1	A	220	ARG	CD-NE-CZ	16.19	147.06	124.40
1	A	194	ARG	NE-CZ-NH1	15.84	137.34	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	HIS	CA-CB-CG	15.68	129.48	113.80
1	A	91	SER	CA-C-N	15.43	137.11	119.98
1	A	91	SER	C-N-CA	15.43	137.11	119.98
1	A	250	ASN	OD1-CG-ND2	-15.42	107.18	122.60
1	A	174	GLU	CA-C-N	14.22	139.78	120.44
1	A	174	GLU	C-N-CA	14.22	139.78	120.44
1	A	172	ARG	NE-CZ-NH1	-13.97	107.53	121.50
1	A	94	ARG	O-C-N	13.52	136.15	122.09
1	A	383	MET	CA-C-N	13.46	135.21	121.35
1	A	383	MET	C-N-CA	13.46	135.21	121.35
1	A	172	ARG	NH1-CZ-NH2	13.15	136.40	119.30
1	A	266	ARG	NE-CZ-NH2	-13.08	107.43	119.20
1	A	175	GLN	CA-C-O	-12.55	107.78	120.70
1	A	299	ALA	O-C-N	-12.32	109.38	122.07
1	C	131	GLY	CA-C-O	-12.30	111.19	121.77
1	A	102	GLN	OE1-CD-NE2	12.14	134.74	122.60
1	A	299	ALA	CA-C-N	11.96	136.76	120.38
1	A	299	ALA	C-N-CA	11.96	136.76	120.38
1	B	250	ASN	OD1-CG-ND2	-11.89	110.71	122.60
1	B	41	ARG	CD-NE-CZ	11.67	140.74	124.40
1	B	220	ARG	CD-NE-CZ	11.57	140.60	124.40
1	A	80	ALA	CA-C-O	-11.46	108.92	121.99
1	D	250	ASN	CA-CB-CG	11.37	123.97	112.60
1	A	265	SER	O-C-N	-11.30	110.34	122.09
1	B	266	ARG	NE-CZ-NH2	-11.30	109.03	119.20
1	B	24	ASN	CA-CB-CG	-11.28	101.32	112.60
1	B	4	SER	CA-C-O	-11.27	101.64	120.80
1	C	94	ARG	CD-NE-CZ	11.25	140.15	124.40
1	A	244	GLY	O-C-N	-11.17	111.47	122.19
1	A	64	GLN	CA-C-O	-11.13	108.23	120.92
1	A	8	ALA	O-C-N	-11.03	107.66	122.43
1	B	5	ILE	CB-CG1-CD1	10.90	136.68	113.80
1	A	180	VAL	CA-C-O	-10.89	109.30	120.85
1	D	200	VAL	N-CA-CB	10.88	126.45	111.21
1	B	101	GLN	OE1-CD-NE2	10.79	133.39	122.60
1	B	359	ASN	CA-C-O	10.75	132.90	121.07
1	C	284	ASP	CA-CB-CG	10.58	123.18	112.60
1	B	322	GLN	CB-CG-CD	10.58	130.58	112.60
1	A	266	ARG	NH1-CZ-NH2	10.55	133.01	119.30
1	A	41	ARG	NE-CZ-NH2	-10.51	109.74	119.20
1	A	270	GLN	OE1-CD-NE2	-10.47	112.13	122.60
1	B	129	ARG	NE-CZ-NH1	-10.42	111.08	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	ALA	O-C-N	-10.37	109.67	123.15
1	B	250	ASN	CB-CG-ND2	10.37	131.95	116.40
1	A	79	GLU	CA-C-O	10.34	131.86	119.97
1	A	346	ILE	CA-C-O	10.32	131.40	120.25
1	B	302	ARG	CD-NE-CZ	10.24	138.74	124.40
1	A	228	MET	CB-CA-C	-10.21	94.85	110.88
1	D	141	ASP	CA-C-O	-10.18	108.51	120.62
1	A	228	MET	CA-CB-CG	10.14	134.38	114.10
1	A	42	ALA	N-CA-CB	-10.03	95.91	110.56
1	A	35	ILE	CA-C-O	10.02	131.37	120.95
1	A	339	VAL	N-CA-CB	-9.96	93.62	110.65
1	A	347	GLY	O-C-N	-9.95	113.90	123.35
1	A	176	ASP	O-C-N	-9.94	111.59	122.12
1	A	152	PHE	CA-CB-CG	-9.93	103.87	113.80
1	A	240	THR	N-CA-CB	-9.93	93.71	110.49
1	D	316	ASN	CA-CB-CG	-9.90	102.70	112.60
1	C	141	ASP	CA-C-O	-9.90	109.41	120.60
1	A	264	ALA	O-C-N	-9.89	111.80	122.09
1	A	42	ALA	CA-C-N	9.89	138.57	120.87
1	A	42	ALA	C-N-CA	9.89	138.57	120.87
1	A	158	GLY	O-C-N	-9.88	111.77	122.24
1	B	158	GLY	CA-C-O	9.87	130.47	120.80
1	B	54	LEU	CA-C-O	-9.86	109.72	120.36
1	A	79	GLU	O-C-N	-9.79	110.23	122.27
1	C	76	VAL	N-CA-C	-9.78	99.37	108.95
1	B	314	GLU	CA-C-O	-9.74	110.04	120.46
1	A	371	ARG	NE-CZ-NH2	-9.74	110.44	119.20
1	A	41	ARG	NE-CZ-NH1	9.69	131.19	121.50
1	C	274	ARG	CD-NE-CZ	9.67	137.94	124.40
1	B	39	LEU	CA-C-O	9.66	130.65	120.70
1	B	338	ASN	OD1-CG-ND2	9.64	132.24	122.60
1	A	8	ALA	CA-C-O	9.63	131.23	119.38
1	A	188	ALA	CA-C-O	-9.63	110.34	120.55
1	A	226	ASP	O-C-N	-9.62	111.79	122.08
1	A	68	ARG	NE-CZ-NH2	-9.58	110.58	119.20
1	A	274	ARG	CD-NE-CZ	9.57	137.79	124.40
1	A	36	SER	O-C-N	-9.56	111.98	122.12
1	A	207	ARG	N-CA-C	-9.54	100.52	112.72
1	A	250	ASN	N-CA-C	9.53	121.89	108.74
1	B	358	LEU	CB-CA-C	-9.52	95.93	110.88
1	C	112	VAL	N-CA-CB	9.50	124.17	111.25
1	A	341	GLY	CA-C-O	-9.48	115.69	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	MET	CA-C-O	9.45	130.74	120.82
1	B	266	ARG	NE-CZ-NH1	9.43	130.93	121.50
1	B	52	VAL	N-CA-CB	9.39	122.20	111.21
1	A	303	ALA	CA-C-N	9.32	139.67	121.41
1	A	303	ALA	C-N-CA	9.32	139.67	121.41
1	A	60	ALA	CA-C-O	9.28	131.07	120.96
1	A	94	ARG	CA-C-O	-9.27	110.98	120.90
1	B	187	GLU	CB-CG-CD	-9.27	96.85	112.60
1	C	348	HIS	N-CA-CB	-9.22	99.52	111.23
1	B	183	GLN	OE1-CD-NE2	-9.22	113.38	122.60
1	B	120	SER	CA-C-O	-9.20	110.67	120.42
1	A	270	GLN	CG-CD-NE2	9.19	130.19	116.40
1	B	378	CYS	O-C-N	-9.18	112.51	123.16
1	A	196	LYS	N-CA-C	9.17	122.25	111.71
1	B	277	SER	CA-C-O	-9.13	111.03	121.26
1	A	12	ARG	NE-CZ-NH1	9.11	130.61	121.50
1	A	166	LYS	CA-C-O	9.10	130.55	121.00
1	A	320	ALA	N-CA-CB	9.09	125.86	110.49
1	A	379	ILE	O-C-N	-9.05	113.42	123.20
1	B	318	ALA	N-CA-CB	9.00	123.05	109.91
1	B	356	ARG	NE-CZ-NH1	-8.97	112.53	121.50
1	D	41	ARG	NH1-CZ-NH2	-8.96	107.64	119.30
1	B	306	LYS	CA-C-O	-8.96	110.61	121.36
1	B	76	VAL	N-CA-C	-8.92	100.73	109.02
1	A	22	PHE	CA-CB-CG	8.87	122.67	113.80
1	A	383	MET	O-C-N	-8.86	113.95	123.26
1	B	76	VAL	CB-CA-C	8.84	119.67	111.00
1	A	326	VAL	CA-CB-CG2	8.84	125.43	110.40
1	A	199	ILE	CA-CB-CG2	8.84	125.52	110.50
1	B	21	ALA	CA-C-O	8.84	130.17	120.63
1	A	198	GLU	N-CA-CB	-8.79	96.66	110.28
1	B	240	THR	N-CA-CB	-8.78	97.10	111.06
1	B	172	ARG	NE-CZ-NH1	-8.77	112.73	121.50
1	A	312	LEU	CA-C-O	-8.75	111.19	120.99
1	B	35	ILE	CB-CA-C	-8.75	100.33	112.14
1	B	55	GLY	N-CA-C	-8.74	100.86	112.14
1	A	284	ASP	O-C-N	-8.73	113.72	121.31
1	B	49	VAL	CA-C-O	-8.73	111.09	121.04
1	A	194	ARG	NE-CZ-NH2	-8.70	111.37	119.20
1	B	158	GLY	O-C-N	-8.68	113.75	122.17
1	A	318	ALA	CA-C-O	8.67	129.93	120.82
1	B	277	SER	O-C-N	8.65	131.39	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	ILE	CA-C-N	-8.63	112.72	122.48
1	B	5	ILE	C-N-CA	-8.63	112.72	122.48
1	B	111	ILE	CB-CG1-CD1	8.62	131.90	113.80
1	A	145	LYS	O-C-N	8.62	130.95	122.07
1	B	353	SER	CA-C-O	-8.62	111.27	120.92
1	B	52	VAL	CA-C-O	-8.59	111.22	120.59
1	A	111	ILE	CA-C-O	-8.55	110.03	121.32
1	A	321	ALA	O-C-N	-8.55	112.93	122.08
1	A	188	ALA	O-C-N	8.53	131.16	122.12
1	B	296	SER	N-CA-CB	8.52	122.78	110.16
1	A	176	ASP	CA-C-O	8.52	129.58	120.55
1	A	86	ASN	OD1-CG-ND2	-8.52	114.08	122.60
1	C	4	SER	CA-C-O	-8.51	106.33	120.80
1	A	11	ALA	CA-C-O	8.50	130.27	120.75
1	B	138	LYS	CA-C-N	8.50	133.73	122.42
1	B	138	LYS	C-N-CA	8.50	133.73	122.42
1	A	168	TRP	N-CA-C	-8.49	102.47	113.17
1	A	269	ILE	CB-CG1-CD1	-8.49	95.98	113.80
1	A	145	LYS	CA-C-O	-8.48	111.92	120.82
1	B	49	VAL	CG1-CB-CG2	-8.48	92.15	110.80
1	B	236	ASP	CA-CB-CG	8.46	121.06	112.60
1	B	381	GLY	N-CA-C	-8.45	103.93	114.92
1	B	152	PHE	CA-CB-CG	-8.45	105.36	113.80
1	A	199	ILE	CB-CA-C	-8.44	100.18	111.15
1	C	156	HIS	CA-CB-CG	8.43	122.23	113.80
1	A	322	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	A	55	GLY	N-CA-C	-8.40	100.12	111.54
1	B	375	ALA	N-CA-CB	-8.39	96.22	110.83
1	B	283	VAL	N-CA-CB	8.37	121.94	112.32
1	C	314	GLU	N-CA-CB	8.36	123.54	110.84
1	A	276	VAL	CA-C-O	-8.35	110.35	119.20
1	D	14	ALA	N-CA-CB	-8.31	98.20	110.17
1	B	300	LEU	CA-C-O	8.29	129.21	120.42
1	A	255	ALA	N-CA-C	8.29	119.58	108.38
1	B	155	TYR	CA-CB-CG	8.27	128.79	113.90
1	B	192	ASP	O-C-N	-8.26	110.37	122.43
1	A	263	GLU	CA-C-O	-8.25	111.72	120.55
1	B	31	GLY	CA-C-O	-8.24	111.50	120.40
1	D	41	ARG	NE-CZ-NH1	8.23	129.73	121.50
1	B	28	HIS	CA-C-O	-8.22	110.81	120.10
1	B	328	LYS	N-CA-CB	8.21	121.92	110.01
1	C	64	GLN	OE1-CD-NE2	8.20	130.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	VAL	CA-C-N	8.19	131.09	120.44
1	A	96	VAL	C-N-CA	8.19	131.09	120.44
1	A	297	ARG	CA-C-N	-8.18	108.68	120.29
1	A	297	ARG	C-N-CA	-8.18	108.68	120.29
1	A	99	GLY	N-CA-C	-8.17	102.42	113.37
1	A	383	MET	CA-C-O	8.15	130.02	121.38
1	C	367	ARG	CD-NE-CZ	8.14	135.80	124.40
1	A	340	ASN	CA-CB-CG	-8.10	104.50	112.60
1	A	365	MET	CA-C-N	8.09	137.00	121.54
1	A	365	MET	C-N-CA	8.09	137.00	121.54
1	B	187	GLU	CA-C-O	8.08	129.30	120.82
1	A	207	ARG	CD-NE-CZ	8.08	135.71	124.40
1	A	247	SER	CA-CB-OG	-8.07	94.96	111.10
1	A	290	THR	CA-CB-OG1	-8.07	97.50	109.60
1	B	96	VAL	CA-C-N	8.05	130.90	120.44
1	B	96	VAL	C-N-CA	8.05	130.90	120.44
1	B	91	SER	N-CA-C	8.03	120.75	111.11
1	A	174	GLU	N-CA-CB	-8.03	98.28	110.16
1	C	280	THR	CA-CB-OG1	-8.01	97.58	109.60
1	A	9	SER	O-C-N	-8.00	115.54	123.46
1	B	264	ALA	CA-C-O	8.00	130.38	121.02
1	A	241	VAL	CA-C-O	-7.96	112.05	120.57
1	B	16	GLY	O-C-N	-7.95	111.28	123.13
1	A	302	ARG	NE-CZ-NH2	-7.93	112.07	119.20
1	A	227	SER	CA-C-O	7.92	129.05	120.10
1	D	98	LEU	CA-C-O	-7.91	112.04	120.42
1	A	124	HIS	CB-CG-CD2	7.90	141.47	131.20
1	B	134	MET	CA-C-O	-7.90	111.90	120.75
1	D	94	ARG	NE-CZ-NH2	7.90	126.31	119.20
1	B	78	GLN	OE1-CD-NE2	-7.90	114.70	122.60
1	B	200	VAL	N-CA-C	-7.89	99.29	107.89
1	B	212	THR	CA-CB-OG1	-7.89	97.76	109.60
1	A	362	LEU	N-CA-C	7.88	119.87	111.28
1	A	177	ALA	O-C-N	-7.88	113.95	122.07
1	C	368	ARG	NE-CZ-NH2	7.87	126.28	119.20
1	B	142	THR	CA-C-O	-7.86	109.71	119.38
1	D	150	ASP	CA-CB-CG	-7.86	104.74	112.60
1	A	91	SER	N-CA-C	7.86	120.54	111.11
1	A	175	GLN	O-C-N	7.85	130.57	122.09
1	C	315	ALA	CB-CA-C	7.85	123.38	110.74
1	A	29	GLU	CB-CG-CD	7.83	125.90	112.60
1	B	359	ASN	OD1-CG-ND2	-7.82	114.78	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	LYS	N-CA-CB	-7.81	98.61	110.16
1	A	95	ALA	CA-C-O	-7.79	112.56	120.90
1	A	327	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	25	THR	CA-C-N	7.78	127.82	119.89
1	A	25	THR	C-N-CA	7.78	127.82	119.89
1	B	298	LYS	CA-CB-CG	7.76	129.62	114.10
1	A	155	TYR	O-C-N	7.75	133.75	122.97
1	B	384	GLY	O-C-N	-7.74	116.96	123.23
1	A	5	ILE	CA-C-O	7.74	127.91	120.25
1	B	221	HIS	CA-C-N	7.73	131.79	120.11
1	B	221	HIS	C-N-CA	7.73	131.79	120.11
1	A	315	ALA	CA-C-O	-7.71	111.91	120.70
1	B	339	VAL	CA-CB-CG2	7.70	123.50	110.40
1	B	142	THR	CA-C-N	7.69	130.90	120.44
1	B	142	THR	C-N-CA	7.69	130.90	120.44
1	B	297	ARG	CA-C-O	-7.68	112.76	120.82
1	B	315	ALA	CA-C-O	-7.66	110.92	120.57
1	A	155	TYR	CA-C-O	-7.66	111.98	121.78
1	B	182	SER	CB-CA-C	-7.66	98.81	110.90
1	A	143	MET	CA-C-O	-7.65	111.75	120.24
1	B	351	GLY	O-C-N	-7.64	114.14	122.24
1	B	353	SER	CA-CB-OG	-7.64	95.82	111.10
1	A	306	LYS	CA-C-O	-7.63	112.33	120.80
1	B	172	ARG	NH1-CZ-NH2	7.63	129.22	119.30
1	A	296	SER	CA-C-O	7.62	128.50	120.42
1	A	166	LYS	O-C-N	-7.61	114.12	122.03
1	D	41	ARG	CD-NE-CZ	7.61	135.05	124.40
1	A	359	ASN	OD1-CG-ND2	7.60	130.20	122.60
1	B	41	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	B	245	ASN	CA-CB-CG	7.58	120.19	112.60
1	A	14	ALA	CA-C-N	-7.58	112.59	122.37
1	A	14	ALA	C-N-CA	-7.58	112.59	122.37
1	B	107	ASP	CA-CB-CG	-7.58	105.02	112.60
1	A	149	THR	CA-C-O	-7.58	112.60	121.16
1	C	279	ALA	N-CA-CB	7.57	123.29	111.56
1	A	86	ASN	CB-CG-ND2	7.57	127.75	116.40
1	B	333	ASP	CA-C-O	7.56	126.98	119.49
1	B	162	GLU	N-CA-CB	7.56	120.97	110.01
1	C	87	GLN	N-CA-C	-7.56	101.21	110.88
1	A	356	ARG	NE-CZ-NH1	-7.55	113.95	121.50
1	A	239	GLY	O-C-N	-7.54	112.90	122.70
1	A	235	PHE	CA-CB-CG	-7.54	106.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	O-C-N	-7.54	114.26	122.85
1	B	64	GLN	OE1-CD-NE2	-7.53	115.07	122.60
1	D	249	LEU	CA-C-O	7.49	128.60	120.43
1	A	122	ALA	O-C-N	7.49	129.82	121.43
1	B	100	MET	O-C-N	-7.49	114.35	122.07
1	A	34	VAL	CA-CB-CG2	-7.49	97.67	110.40
1	A	256	ALA	CA-C-O	-7.47	112.40	121.06
1	B	34	VAL	CA-C-O	-7.46	112.94	120.85
1	B	367	ARG	O-C-N	-7.45	114.22	122.12
1	B	20	GLY	O-C-N	-7.44	113.03	122.70
1	B	358	LEU	O-C-N	-7.43	114.41	122.07
1	D	200	VAL	CA-CB-CG1	7.43	123.04	110.40
1	D	207	ARG	CD-NE-CZ	7.43	134.80	124.40
1	A	111	ILE	O-C-N	7.42	130.83	123.03
1	A	232	ARG	CA-CB-CG	7.40	128.90	114.10
1	C	133	LYS	N-CA-CB	7.40	121.69	110.30
1	A	309	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	69	GLN	O-C-N	-7.39	114.28	122.12
1	A	371	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	C	4	SER	CA-CB-OG	7.39	125.87	111.10
1	A	58	LEU	CA-C-N	7.38	129.82	120.89
1	A	58	LEU	C-N-CA	7.38	129.82	120.89
1	C	214	ASP	CA-CB-CG	7.38	119.98	112.60
1	B	166	LYS	N-CA-CB	7.38	121.03	109.82
1	C	279	ALA	O-C-N	7.36	131.29	123.42
1	A	311	ASP	CA-CB-CG	-7.36	105.24	112.60
1	B	157	MET	CA-C-N	7.35	128.26	120.03
1	B	157	MET	C-N-CA	7.35	128.26	120.03
1	C	163	ASN	CA-CB-CG	7.34	119.94	112.60
1	D	251	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	65	ASN	O-C-N	-7.31	112.91	121.32
1	A	231	LEU	CD1-CG-CD2	7.31	126.88	110.80
1	D	127	HIS	O-C-N	-7.30	114.73	123.13
1	B	174	GLU	CB-CG-CD	7.30	125.01	112.60
1	A	4	SER	CA-CB-OG	7.29	125.69	111.10
1	A	379	ILE	CA-C-N	7.29	135.70	121.41
1	A	379	ILE	C-N-CA	7.29	135.70	121.41
1	D	338	ASN	CA-C-O	7.28	130.16	121.65
1	A	180	VAL	O-C-N	7.27	129.32	121.83
1	C	367	ARG	NE-CZ-NH2	-7.27	112.66	119.20
1	B	245	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	A	138	LYS	CA-C-N	7.26	132.27	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	LYS	C-N-CA	7.26	132.27	122.84
1	C	381	GLY	N-CA-C	-7.26	105.49	114.92
1	A	30	LEU	CA-C-N	-7.25	107.89	120.79
1	A	30	LEU	C-N-CA	-7.25	107.89	120.79
1	A	12	ARG	NE-CZ-NH2	-7.25	112.68	119.20
1	C	370	ALA	CA-C-O	-7.24	113.14	121.47
1	A	227	SER	O-C-N	-7.23	113.76	122.22
1	B	100	MET	CA-C-N	7.22	129.95	120.28
1	B	100	MET	C-N-CA	7.22	129.95	120.28
1	A	9	SER	CA-C-O	7.22	129.04	121.10
1	A	297	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	B	144	ILE	CB-CG1-CD1	7.21	128.94	113.80
1	C	207	ARG	CD-NE-CZ	7.20	134.47	124.40
1	C	133	LYS	CA-C-O	-7.19	111.30	119.79
1	A	22	PHE	CA-C-O	7.19	128.43	119.95
1	D	231	LEU	N-CA-CB	7.18	120.51	110.17
1	D	254	ALA	CB-CA-C	7.17	123.29	110.16
1	A	356	ARG	NE-CZ-NH2	7.15	125.64	119.20
1	B	367	ARG	CD-NE-CZ	7.15	134.41	124.40
1	B	385	VAL	O-C-N	-7.14	115.46	123.10
1	C	283	VAL	N-CA-CB	7.14	123.02	111.23
1	A	197	ASP	CA-C-N	7.14	131.16	120.31
1	A	197	ASP	C-N-CA	7.14	131.16	120.31
1	B	196	LYS	N-CA-CB	-7.14	99.22	110.28
1	B	295	ALA	CA-C-O	-7.12	112.87	120.42
1	C	157	MET	O-C-N	-7.12	114.68	122.09
1	B	371	ARG	CA-C-O	-7.12	111.17	119.78
1	B	36	SER	CA-CB-OG	7.12	125.33	111.10
1	B	300	LEU	O-C-N	-7.11	114.05	122.15
1	D	122	ALA	CA-C-O	7.10	126.90	119.80
1	B	126	ALA	CB-CA-C	-7.09	97.90	109.89
1	B	160	THR	N-CA-CB	7.09	121.14	110.22
1	D	13	THR	N-CA-CB	7.09	121.34	110.49
1	C	103	ILE	N-CA-CB	7.09	120.72	110.52
1	B	246	ALA	CA-C-O	-7.08	112.72	121.78
1	B	259	MET	O-C-N	7.07	130.68	123.26
1	A	350	ILE	CA-CB-CG1	7.06	122.40	110.40
1	B	124	HIS	O-C-N	-7.06	114.27	123.16
1	A	8	ALA	N-CA-CB	-7.05	98.68	110.39
1	B	44	VAL	CG1-CB-CG2	-7.04	95.30	110.80
1	A	11	ALA	O-C-N	-7.04	116.10	123.56
1	B	44	VAL	CA-C-N	-7.04	107.92	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	VAL	C-N-CA	-7.04	107.92	122.07
1	B	129	ARG	NH1-CZ-NH2	7.04	128.45	119.30
1	B	169	GLN	CB-CG-CD	7.03	124.55	112.60
1	A	359	ASN	CA-C-O	7.01	128.19	120.82
1	B	270	GLN	O-C-N	7.01	128.26	120.83
1	C	131	GLY	CA-C-N	-7.01	113.93	122.90
1	C	131	GLY	C-N-CA	-7.01	113.93	122.90
1	B	392	LEU	N-CA-CB	7.01	122.41	110.50
1	C	107	ASP	CA-CB-CG	-7.01	105.59	112.60
1	D	231	LEU	CD1-CG-CD2	-7.00	95.40	110.80
1	A	288	MET	CA-C-N	6.99	133.24	120.79
1	A	288	MET	C-N-CA	6.99	133.24	120.79
1	A	346	ILE	N-CA-C	6.98	120.80	111.44
1	D	55	GLY	N-CA-C	-6.98	102.60	112.37
1	B	364	GLU	O-C-N	-6.98	113.16	122.23
1	B	23	ALA	O-C-N	-6.97	113.32	122.59
1	A	30	LEU	O-C-N	6.96	130.09	122.15
1	D	172	ARG	NE-CZ-NH1	6.95	128.45	121.50
1	B	339	VAL	CA-C-O	-6.95	111.23	119.85
1	C	68	ARG	NH1-CZ-NH2	6.95	128.33	119.30
1	A	40	GLU	CB-CG-CD	6.93	124.38	112.60
1	C	339	VAL	CB-CA-C	6.93	121.49	112.14
1	A	342	GLY	O-C-N	6.93	131.71	122.70
1	A	75	GLY	CA-C-O	-6.92	111.10	119.06
1	A	241	VAL	O-C-N	6.92	130.71	123.03
1	D	22	PHE	CA-C-N	6.89	134.70	121.54
1	D	22	PHE	C-N-CA	6.89	134.70	121.54
1	D	361	LEU	CB-CA-C	-6.89	99.79	110.81
1	D	225	LEU	CD1-CG-CD2	-6.88	95.66	110.80
1	B	216	ASP	CB-CG-OD1	6.88	134.22	118.40
1	A	263	GLU	CG-CD-OE1	6.87	134.20	118.40
1	C	69	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	A	43	GLY	CA-C-O	6.87	128.09	119.72
1	B	245	ASN	CB-CA-C	6.87	122.16	110.56
1	A	228	MET	O-C-N	-6.86	115.00	122.07
1	B	318	ALA	CB-CA-C	-6.85	100.41	110.96
1	B	338	ASN	O-C-N	-6.85	114.06	122.55
1	D	48	GLU	CA-C-N	6.84	130.42	120.91
1	D	48	GLU	C-N-CA	6.84	130.42	120.91
1	A	322	GLN	CB-CG-CD	6.84	124.23	112.60
1	B	376	THR	CA-C-O	-6.83	112.14	120.54
1	A	358	LEU	CA-C-O	6.83	127.66	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	LEU	N-CA-CB	-6.82	100.17	111.49
1	B	377	LEU	CA-C-N	6.82	132.18	122.09
1	B	377	LEU	C-N-CA	6.82	132.18	122.09
1	A	215	ALA	CA-C-N	6.81	134.54	121.54
1	A	215	ALA	C-N-CA	6.81	134.54	121.54
1	B	329	ASP	CA-C-O	6.81	127.71	120.70
1	C	353	SER	CA-C-O	-6.81	112.58	120.20
1	A	43	GLY	O-C-N	-6.80	115.06	122.41
1	B	14	ALA	CA-C-N	-6.80	113.59	122.37
1	B	14	ALA	C-N-CA	-6.80	113.59	122.37
1	A	30	LEU	CA-C-O	-6.80	113.21	120.42
1	A	44	VAL	CA-C-O	6.79	127.68	120.48
1	A	261	GLU	CA-C-N	6.79	130.63	120.31
1	A	261	GLU	C-N-CA	6.79	130.63	120.31
1	B	172	ARG	CA-C-O	6.77	128.52	121.07
1	C	321	ALA	CA-C-O	-6.77	113.66	120.90
1	C	14	ALA	N-CA-C	-6.77	101.60	110.53
1	A	367	ARG	O-C-N	-6.76	114.95	122.12
1	A	316	ASN	CA-CB-CG	-6.76	105.84	112.60
1	B	183	GLN	CG-CD-OE1	6.74	134.28	120.80
1	A	214	ASP	CA-C-O	6.74	126.52	119.51
1	B	68	ARG	NH1-CZ-NH2	-6.73	110.55	119.30
1	B	176	ASP	O-C-N	-6.72	115.00	122.12
1	A	39	LEU	CA-C-N	6.72	129.28	120.28
1	A	39	LEU	C-N-CA	6.72	129.28	120.28
1	A	184	ASN	O-C-N	-6.71	115.01	122.12
1	B	77	PRO	O-C-N	-6.71	114.80	122.91
1	B	153	TYR	CA-CB-CG	-6.70	101.85	113.90
1	C	235	PHE	CA-CB-CG	-6.70	107.10	113.80
1	B	220	ARG	NE-CZ-NH1	6.69	128.19	121.50
1	A	173	ASP	CA-C-O	6.67	127.62	120.55
1	B	5	ILE	CB-CA-C	-6.67	100.76	110.63
1	C	18	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	310	LEU	CA-C-O	-6.66	114.50	121.55
1	C	104	ALA	CA-C-O	-6.64	113.52	120.55
1	A	139	MET	CA-C-O	-6.63	113.64	120.54
1	A	17	SER	O-C-N	-6.62	115.47	122.96
1	D	139	MET	CA-C-N	-6.62	113.83	122.37
1	D	139	MET	C-N-CA	-6.62	113.83	122.37
1	A	250	ASN	CB-CG-ND2	6.61	126.32	116.40
1	A	317	GLU	CA-C-O	-6.61	114.11	122.63
1	A	52	VAL	N-CA-CB	6.60	118.94	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	A	253	ALA	CA-C-O	-6.60	114.20	121.33
1	D	50	ASN	OD1-CG-ND2	6.60	129.20	122.60
1	B	77	PRO	N-CA-CB	6.60	109.59	103.39
1	B	187	GLU	CA-CB-CG	-6.59	100.92	114.10
1	B	68	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	A	321	ALA	CA-C-N	6.58	129.64	120.29
1	A	321	ALA	C-N-CA	6.58	129.64	120.29
1	A	258	LEU	N-CA-C	6.58	120.33	110.14
1	A	316	ASN	CA-C-O	6.57	128.17	121.07
1	A	299	ALA	CA-C-O	6.57	127.72	120.82
1	C	144	ILE	CB-CA-C	-6.57	103.44	112.24
1	B	64	GLN	N-CA-C	6.57	119.74	109.96
1	B	271	PRO	CA-C-O	-6.57	113.98	122.12
1	B	361	LEU	CA-C-N	6.55	129.06	120.28
1	B	361	LEU	C-N-CA	6.55	129.06	120.28
1	D	103	ILE	CA-C-N	6.55	129.72	120.28
1	D	103	ILE	C-N-CA	6.55	129.72	120.28
1	C	327	ASN	CA-CB-CG	6.54	119.14	112.60
1	B	181	ALA	O-C-N	-6.53	114.23	122.27
1	A	173	ASP	N-CA-C	6.53	118.40	111.28
1	B	111	ILE	CB-CA-C	-6.52	100.91	110.62
1	D	4	SER	CA-C-O	-6.52	109.72	120.80
1	B	250	ASN	O-C-N	-6.51	114.75	122.96
1	B	258	LEU	O-C-N	-6.51	114.72	123.19
1	C	131	GLY	N-CA-C	-6.51	103.19	111.72
1	B	350	ILE	N-CA-C	6.51	122.88	109.34
1	C	98	LEU	CA-C-N	6.50	127.15	120.00
1	C	98	LEU	C-N-CA	6.50	127.15	120.00
1	B	192	ASP	CA-C-N	6.50	131.39	121.51
1	B	192	ASP	C-N-CA	6.50	131.39	121.51
1	C	293	ILE	CA-C-N	6.50	126.27	119.05
1	C	293	ILE	C-N-CA	6.50	126.27	119.05
1	B	318	ALA	N-CA-C	-6.50	103.89	110.97
1	B	243	ALA	N-CA-CB	-6.50	100.21	110.28
1	C	55	GLY	N-CA-C	-6.48	100.14	111.62
1	B	43	GLY	N-CA-C	-6.47	105.11	115.08
1	D	124	HIS	CA-CB-CG	6.47	120.27	113.80
1	D	133	LYS	N-CA-C	6.47	118.34	111.28
1	B	382	GLY	O-C-N	-6.47	114.29	122.70
1	B	102	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	C	109	SER	CB-CA-C	-6.46	99.93	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	GLN	O-C-N	6.46	130.78	123.42
1	A	109	SER	CA-CB-OG	-6.46	98.19	111.10
1	B	36	SER	CA-C-O	-6.46	113.58	120.42
1	A	104	ALA	N-CA-CB	6.45	119.60	110.12
1	A	166	LYS	CB-CG-CD	6.44	126.11	111.30
1	A	339	VAL	CA-CB-CG2	6.44	121.34	110.40
1	B	264	ALA	O-C-N	-6.43	114.42	122.20
1	B	194	ARG	CB-CG-CD	6.43	126.08	111.30
1	A	157	MET	CA-C-N	6.42	128.16	120.14
1	A	157	MET	C-N-CA	6.42	128.16	120.14
1	A	381	GLY	N-CA-C	-6.42	106.58	114.92
1	C	338	ASN	CA-C-O	6.41	130.09	122.14
1	B	110	ILE	O-C-N	-6.40	116.52	123.18
1	B	145	LYS	CB-CG-CD	6.40	126.02	111.30
1	D	86	ASN	N-CA-C	6.40	118.83	108.34
1	B	160	THR	N-CA-C	-6.40	104.35	111.71
1	B	327	ASN	OD1-CG-ND2	-6.39	116.21	122.60
1	B	271	PRO	O-C-N	6.38	130.93	123.14
1	D	34	VAL	N-CA-CB	-6.38	101.86	110.54
1	D	172	ARG	NH1-CZ-NH2	-6.38	111.00	119.30
1	A	88	LEU	O-C-N	-6.38	114.10	122.59
1	C	68	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	C	200	VAL	N-CA-C	-6.38	100.46	107.73
1	A	297	ARG	O-C-N	6.38	128.64	122.07
1	B	250	ASN	N-CA-C	6.38	118.64	109.14
1	B	143	MET	O-C-N	6.37	128.97	122.09
1	B	187	GLU	O-C-N	-6.36	115.52	122.07
1	A	177	ALA	CA-C-N	6.35	129.11	120.54
1	A	177	ALA	C-N-CA	6.35	129.11	120.54
1	A	220	ARG	NE-CZ-NH2	-6.35	113.49	119.20
1	D	68	ARG	CA-C-O	-6.34	113.69	120.42
1	D	261	GLU	CB-CA-C	-6.34	100.92	110.88
1	D	46	ALA	CA-C-O	6.34	127.48	120.63
1	A	347	GLY	CA-C-N	6.34	129.82	122.85
1	A	347	GLY	C-N-CA	6.34	129.82	122.85
1	C	104	ALA	CB-CA-C	-6.34	100.27	110.79
1	C	327	ASN	CA-C-O	6.33	127.13	120.42
1	A	336	ILE	CA-C-N	-6.33	115.34	123.19
1	A	336	ILE	C-N-CA	-6.33	115.34	123.19
1	A	223	ALA	CB-CA-C	6.33	119.77	109.90
1	B	273	GLY	O-C-N	6.32	130.98	123.46
1	A	78	GLN	CA-C-N	6.32	129.91	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLN	C-N-CA	6.32	129.91	120.31
1	B	21	ALA	O-C-N	-6.31	115.43	122.12
1	C	108	ALA	CA-C-N	6.31	133.51	122.79
1	C	108	ALA	C-N-CA	6.31	133.51	122.79
1	B	120	SER	CB-CA-C	-6.31	100.13	110.85
1	A	239	GLY	CA-C-O	6.30	131.54	120.57
1	A	339	VAL	O-C-N	-6.30	115.50	121.87
1	B	156	HIS	CA-CB-CG	6.30	120.10	113.80
1	C	236	ASP	CA-CB-CG	6.30	118.90	112.60
1	C	371	ARG	CD-NE-CZ	6.30	133.22	124.40
1	B	348	HIS	CA-CB-CG	-6.30	107.50	113.80
1	C	137	PHE	N-CA-C	-6.30	99.50	109.07
1	A	36	SER	CA-C-O	6.29	127.22	120.55
1	A	240	THR	N-CA-C	6.29	124.19	110.80
1	D	77	PRO	CB-CA-C	6.29	119.23	111.12
1	A	364	GLU	N-CA-C	-6.28	103.97	111.69
1	A	102	GLN	CA-C-O	-6.27	112.76	119.97
1	B	6	VAL	CA-C-N	-6.27	115.17	122.95
1	B	6	VAL	C-N-CA	-6.27	115.17	122.95
1	B	319	PHE	CA-C-N	-6.27	111.79	120.38
1	B	319	PHE	C-N-CA	-6.27	111.79	120.38
1	A	227	SER	CA-CB-OG	-6.26	98.57	111.10
1	A	6	VAL	CA-C-N	-6.26	115.19	122.95
1	A	6	VAL	C-N-CA	-6.26	115.19	122.95
1	C	94	ARG	CA-C-O	-6.26	113.91	120.55
1	D	88	LEU	CB-CA-C	-6.25	109.35	116.54
1	D	275	ILE	CB-CG1-CD1	6.25	126.93	113.80
1	A	267	ARG	N-CA-CB	-6.25	100.30	110.42
1	B	367	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	C	83	TRP	CA-C-O	6.25	127.76	120.89
1	C	269	ILE	O-C-N	-6.25	115.35	122.72
1	A	12	ARG	CD-NE-CZ	6.24	133.13	124.40
1	B	249	LEU	O-C-N	-6.23	116.11	123.22
1	A	62	GLU	O-C-N	-6.23	114.08	122.43
1	C	68	ARG	CD-NE-CZ	6.23	133.12	124.40
1	B	78	GLN	CB-CG-CD	6.22	123.18	112.60
1	B	210	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	342	GLY	O-C-N	6.22	130.79	122.70
1	B	337	VAL	CA-C-N	-6.22	113.53	122.36
1	B	337	VAL	C-N-CA	-6.22	113.53	122.36
1	B	172	ARG	CA-C-N	6.21	128.89	120.38
1	B	172	ARG	C-N-CA	6.21	128.89	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	MET	CA-C-N	6.21	128.60	120.28
1	C	119	MET	C-N-CA	6.21	128.60	120.28
1	A	95	ALA	N-CA-CB	6.21	119.19	109.94
1	B	113	ALA	CA-C-N	6.21	133.57	121.41
1	B	113	ALA	C-N-CA	6.21	133.57	121.41
1	B	345	ALA	O-C-N	6.20	130.67	122.30
1	A	243	ALA	N-CA-CB	-6.20	100.67	110.28
1	C	136	ASP	CA-CB-CG	-6.20	106.40	112.60
1	A	158	GLY	CA-C-O	6.20	127.09	120.40
1	B	157	MET	O-C-N	-6.20	114.97	122.22
1	A	49	VAL	CA-C-O	-6.20	113.78	120.85
1	C	53	ILE	CA-C-O	-6.20	113.95	120.39
1	A	350	ILE	CA-CB-CG2	-6.19	99.97	110.50
1	B	367	ARG	NE-CZ-NH1	6.19	127.69	121.50
1	A	29	GLU	CA-C-O	6.18	126.97	120.42
1	A	65	ASN	OD1-CG-ND2	6.18	128.78	122.60
1	A	270	GLN	CB-CA-C	6.18	122.35	110.17
1	C	329	ASP	CA-CB-CG	-6.17	106.43	112.60
1	A	34	VAL	CA-C-O	-6.17	113.59	120.25
1	A	194	ARG	NH1-CZ-NH2	-6.17	111.28	119.30
1	A	143	MET	O-C-N	6.16	130.24	122.23
1	A	78	GLN	CA-CB-CG	-6.16	101.78	114.10
1	A	19	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	144	ILE	CA-C-O	6.16	127.88	121.05
1	B	28	HIS	O-C-N	6.15	129.42	122.22
1	B	221	HIS	O-C-N	-6.15	116.03	123.16
1	A	77	PRO	CA-C-O	6.15	129.63	121.95
1	A	163	ASN	CA-CB-CG	6.15	118.75	112.60
1	C	355	ALA	N-CA-C	-6.14	104.49	112.23
1	B	227	SER	CA-C-O	6.14	126.92	119.49
1	A	13	THR	OG1-CB-CG2	-6.13	97.03	109.30
1	C	308	GLY	CA-C-O	-6.13	114.19	120.45
1	C	243	ALA	N-CA-C	-6.13	104.67	111.36
1	B	254	ALA	CA-C-O	6.13	127.62	120.75
1	D	81	THR	CA-C-O	-6.13	114.47	121.58
1	D	348	HIS	N-CA-CB	-6.13	103.49	111.09
1	B	371	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	B	214	ASP	CA-C-O	6.12	125.88	119.51
1	D	12	ARG	CG-CD-NE	6.11	125.45	112.00
1	B	11	ALA	CB-CA-C	-6.11	100.16	109.99
1	D	368	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	91	SER	O-C-N	-6.10	115.75	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	GLU	CG-CD-OE1	-6.10	104.38	118.40
1	A	18	PHE	CA-C-O	-6.09	114.22	120.80
1	A	150	ASP	N-CA-CB	6.09	119.26	110.06
1	A	269	ILE	N-CA-CB	-6.09	102.15	110.56
1	A	205	LYS	N-CA-CB	6.09	119.13	109.51
1	A	42	ALA	O-C-N	-6.08	115.05	122.34
1	A	210	ASP	CA-C-N	-6.08	115.18	123.14
1	A	210	ASP	C-N-CA	-6.08	115.18	123.14
1	C	104	ALA	N-CA-CB	6.07	119.04	110.12
1	D	251	ASP	CA-C-O	6.06	127.96	121.11
1	B	111	ILE	CA-C-N	-6.06	115.14	122.90
1	B	111	ILE	C-N-CA	-6.06	115.14	122.90
1	C	123	PRO	CA-C-O	6.06	130.15	122.15
1	A	19	ASN	O-C-N	-6.06	114.46	122.40
1	B	112	VAL	CA-C-N	-6.05	113.09	122.59
1	B	112	VAL	C-N-CA	-6.05	113.09	122.59
1	C	132	VAL	CA-C-O	-6.05	114.00	120.59
1	C	114	GLY	CA-C-N	-6.05	111.25	121.47
1	C	114	GLY	C-N-CA	-6.05	111.25	121.47
1	B	240	THR	CB-CA-C	6.04	118.41	109.29
1	A	228	MET	CG-SD-CE	-6.04	87.61	100.90
1	D	133	LYS	CA-CB-CG	6.04	126.17	114.10
1	A	272	LEU	CA-C-O	6.04	126.79	119.31
1	A	13	THR	CA-CB-OG1	6.03	118.65	109.60
1	A	307	ILE	CA-C-O	6.03	128.32	120.78
1	B	361	LEU	CB-CG-CD2	6.03	128.79	110.70
1	A	129	ARG	NE-CZ-NH1	-6.02	115.48	121.50
1	A	129	ARG	NH1-CZ-NH2	6.02	127.12	119.30
1	C	59	PRO	N-CA-CB	-6.01	96.94	103.25
1	C	259	MET	CA-C-O	-6.01	114.85	121.28
1	D	296	SER	CA-C-O	6.01	127.33	120.90
1	D	112	VAL	N-CA-C	-6.01	99.76	108.17
1	A	26	PRO	N-CA-CB	6.01	108.37	103.32
1	A	338	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	B	167	GLN	N-CA-C	6.01	118.60	111.33
1	D	6	VAL	CB-CA-C	-6.01	102.60	111.19
1	B	200	VAL	CA-C-N	6.00	126.31	119.83
1	B	200	VAL	C-N-CA	6.00	126.31	119.83
1	B	198	GLU	N-CA-C	6.00	117.90	111.36
1	C	111	ILE	CA-C-N	-6.00	115.75	123.19
1	C	111	ILE	C-N-CA	-6.00	115.75	123.19
1	C	275	ILE	CA-C-N	-6.00	111.52	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	ILE	C-N-CA	-6.00	111.52	120.82
1	D	79	GLU	CA-CB-CG	-6.00	102.10	114.10
1	B	16	GLY	CA-C-O	6.00	130.58	121.58
1	C	356	ARG	CA-CB-CG	6.00	126.09	114.10
1	A	350	ILE	N-CA-C	5.99	121.80	109.34
1	B	127	HIS	CA-CB-CG	-5.99	107.81	113.80
1	C	367	ARG	CA-C-O	-5.99	113.09	119.97
1	B	353	SER	N-CA-C	5.98	121.24	111.37
1	B	6	VAL	CB-CA-C	-5.98	103.56	111.70
1	B	29	GLU	CG-CD-OE1	5.98	132.16	118.40
1	A	68	ARG	NH1-CZ-NH2	5.98	127.08	119.30
1	B	228	MET	CA-C-O	5.98	126.87	120.24
1	A	122	ALA	CA-C-O	-5.98	113.80	120.25
1	A	256	ALA	O-C-N	5.96	130.19	123.27
1	B	149	THR	CA-C-O	-5.96	113.93	120.43
1	B	302	ARG	CG-CD-NE	5.96	125.11	112.00
1	A	172	ARG	CA-C-N	5.96	128.26	120.28
1	A	172	ARG	C-N-CA	5.96	128.26	120.28
1	A	87	GLN	N-CA-C	-5.95	103.30	110.44
1	C	150	ASP	CA-CB-CG	-5.95	106.65	112.60
1	B	297	ARG	CD-NE-CZ	5.95	132.73	124.40
1	C	344	ILE	CA-C-O	-5.95	114.76	120.95
1	B	260	SER	CA-C-N	5.95	128.74	120.29
1	B	260	SER	C-N-CA	5.95	128.74	120.29
1	B	88	LEU	CD1-CG-CD2	-5.94	97.73	110.80
1	B	195	PHE	O-C-N	-5.94	113.98	122.41
1	A	67	ALA	CA-C-O	5.93	126.84	120.55
1	B	360	THR	CA-CB-OG1	-5.93	100.70	109.60
1	B	339	VAL	N-CA-CB	-5.92	98.61	111.05
1	A	261	GLU	O-C-N	-5.92	115.29	122.22
1	B	155	TYR	CA-C-O	-5.91	114.21	121.78
1	A	369	GLY	CA-C-O	5.91	126.56	119.82
1	D	255	ALA	CA-C-O	5.91	127.64	121.38
1	B	297	ARG	NH1-CZ-NH2	-5.91	111.62	119.30
1	C	133	LYS	O-C-N	5.91	130.25	122.33
1	B	261	GLU	N-CA-C	-5.91	104.92	111.36
1	D	203	ILE	CB-CA-C	-5.90	103.75	111.25
1	B	250	ASN	CA-C-N	5.90	132.29	122.73
1	B	250	ASN	C-N-CA	5.90	132.29	122.73
1	C	33	THR	CA-CB-CG2	5.90	120.52	110.50
1	C	361	LEU	CA-C-N	5.90	128.18	120.28
1	C	361	LEU	C-N-CA	5.90	128.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	SER	CA-CB-OG	-5.89	99.31	111.10
1	A	378	CYS	N-CA-CB	5.89	119.77	110.23
1	B	280	THR	CA-CB-OG1	-5.88	100.78	109.60
1	C	322	GLN	OE1-CD-NE2	5.88	128.48	122.60
1	A	221	HIS	O-C-N	-5.87	116.53	123.22
1	A	339	VAL	CB-CA-C	5.87	121.26	112.16
1	A	117	GLU	CA-C-N	-5.86	114.02	123.23
1	A	117	GLU	C-N-CA	-5.86	114.02	123.23
1	B	160	THR	O-C-N	5.86	129.08	122.22
1	D	145	LYS	O-C-N	5.86	128.36	122.03
1	D	198	GLU	O-C-N	5.86	128.33	122.12
1	A	125	CYS	CA-C-O	-5.86	115.18	121.45
1	D	175	GLN	OE1-CD-NE2	5.86	128.46	122.60
1	B	168	TRP	CA-C-O	-5.85	112.20	119.28
1	B	202	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	230	LYS	N-CA-CB	-5.85	100.59	110.41
1	A	252	GLY	O-C-N	-5.85	116.59	123.55
1	B	70	ALA	CA-C-N	-5.85	112.84	120.44
1	B	70	ALA	C-N-CA	-5.85	112.84	120.44
1	B	235	PHE	CA-CB-CG	-5.84	107.96	113.80
1	C	131	GLY	O-C-N	5.83	127.53	122.64
1	B	173	ASP	CB-CA-C	-5.83	100.78	110.68
1	B	216	ASP	CA-C-N	-5.82	111.85	122.38
1	B	216	ASP	C-N-CA	-5.82	111.85	122.38
1	B	267	ARG	NE-CZ-NH1	5.82	127.32	121.50
1	D	378	CYS	CA-C-O	-5.81	114.35	120.80
1	A	207	ARG	CA-C-O	5.81	126.61	119.81
1	A	65	ASN	CA-C-N	5.80	127.09	119.84
1	A	65	ASN	C-N-CA	5.80	127.09	119.84
1	D	9	SER	CA-CB-OG	-5.80	99.49	111.10
1	D	150	ASP	N-CA-CB	5.80	118.59	109.83
1	A	4	SER	CA-C-O	-5.80	110.94	120.80
1	A	334	PRO	O-C-N	-5.80	114.47	122.24
1	D	124	HIS	N-CA-CB	5.80	120.03	110.69
1	C	132	VAL	CB-CA-C	5.79	118.92	110.98
1	A	64	GLN	N-CA-C	5.79	118.72	110.10
1	B	40	GLU	O-C-N	5.79	128.34	122.09
1	C	274	ARG	CA-C-O	-5.78	114.58	120.71
1	A	124	HIS	CB-CG-ND1	-5.78	114.03	122.70
1	A	386	ALA	CA-C-O	-5.77	114.36	121.06
1	D	140	ILE	N-CA-C	5.77	116.89	108.58
1	B	340	ASN	CB-CG-ND2	5.77	125.05	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	GLN	N-CA-C	-5.77	103.50	110.88
1	C	234	ALA	N-CA-C	5.76	119.49	112.23
1	A	143	MET	N-CA-C	-5.75	104.61	111.69
1	C	267	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	C	357	ILE	CA-C-O	-5.75	114.97	120.95
1	A	239	GLY	CA-C-N	5.75	132.52	121.54
1	A	239	GLY	C-N-CA	5.75	132.52	121.54
1	A	183	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	359	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	218	TYR	N-CA-CB	-5.74	101.46	110.30
1	D	43	GLY	N-CA-C	-5.74	107.06	115.72
1	A	224	THR	N-CA-CB	5.74	119.98	110.63
1	B	228	MET	CA-CB-CG	5.73	125.56	114.10
1	B	278	TRP	CA-CB-CG	-5.73	102.71	113.60
1	D	258	LEU	CA-C-O	5.73	126.78	120.71
1	B	99	GLY	N-CA-C	-5.72	105.44	112.77
1	A	5	ILE	CB-CG1-CD1	5.72	125.81	113.80
1	B	274	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	A	65	ASN	N-CA-C	5.72	122.44	109.81
1	A	211	ILE	CA-C-O	-5.72	114.39	120.39
1	A	115	GLY	CA-C-N	-5.71	111.87	121.75
1	A	115	GLY	C-N-CA	-5.71	111.87	121.75
1	B	28	HIS	CA-CB-CG	-5.71	108.09	113.80
1	A	322	GLN	CA-CB-CG	5.71	125.52	114.10
1	B	224	THR	CA-CB-CG2	-5.71	100.79	110.50
1	A	329	ASP	CB-CA-C	-5.71	101.88	110.90
1	A	223	ALA	O-C-N	-5.71	115.88	122.95
1	A	103	ILE	CA-C-N	5.70	127.92	120.28
1	A	103	ILE	C-N-CA	5.70	127.92	120.28
1	A	167	GLN	CA-C-N	-5.70	113.14	122.54
1	A	167	GLN	C-N-CA	-5.70	113.14	122.54
1	A	129	ARG	CG-CD-NE	-5.70	99.47	112.00
1	A	247	SER	CA-C-O	-5.70	115.54	121.98
1	B	142	THR	N-CA-CB	5.70	119.84	110.39
1	B	266	ARG	O-C-N	-5.70	116.08	122.12
1	B	101	GLN	O-C-N	-5.69	116.08	122.12
1	A	379	ILE	N-CA-CB	-5.69	103.21	111.52
1	C	146	ASP	CA-CB-CG	-5.69	106.91	112.60
1	A	356	ARG	O-C-N	-5.68	116.09	122.12
1	A	196	LYS	N-CA-CB	-5.68	101.47	110.22
1	B	313	VAL	CA-C-N	-5.68	115.05	123.11
1	B	313	VAL	C-N-CA	-5.68	115.05	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	HIS	N-CA-CB	-5.67	101.38	110.63
1	A	384	GLY	N-CA-C	5.67	119.41	110.96
1	A	38	VAL	CA-C-O	5.67	126.59	120.47
1	A	112	VAL	CA-C-N	-5.67	113.69	122.59
1	A	112	VAL	C-N-CA	-5.67	113.69	122.59
1	A	224	THR	OG1-CB-CG2	-5.66	97.97	109.30
1	B	157	MET	CA-C-O	5.66	126.50	120.10
1	B	219	ILE	N-CA-CB	5.66	117.71	110.13
1	C	140	ILE	N-CA-CB	-5.66	104.37	110.53
1	B	4	SER	CB-CA-C	5.65	120.84	110.10
1	B	349	PRO	CB-CA-C	5.65	120.89	111.56
1	C	241	VAL	O-C-N	5.65	129.31	123.03
1	A	234	ALA	N-CA-CB	-5.65	102.22	110.53
1	B	47	GLY	CA-C-N	5.65	132.57	122.06
1	B	47	GLY	C-N-CA	5.65	132.57	122.06
1	C	134	MET	CB-CA-C	5.65	120.03	109.86
1	D	333	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	194	ARG	NH1-CZ-NH2	-5.64	111.97	119.30
1	B	290	THR	CA-CB-OG1	-5.64	101.14	109.60
1	A	359	ASN	CB-CG-OD1	-5.64	109.52	120.80
1	A	55	GLY	CA-C-O	5.64	126.65	121.58
1	B	12	ARG	CA-C-O	-5.64	115.24	121.33
1	C	17	SER	CA-CB-OG	5.64	122.37	111.10
1	A	361	LEU	CB-CA-C	-5.63	102.03	110.88
1	A	260	SER	CA-C-N	5.63	128.38	120.28
1	A	260	SER	C-N-CA	5.63	128.38	120.28
1	B	348	HIS	N-CA-C	5.63	118.32	108.75
1	A	253	ALA	O-C-N	5.62	129.66	123.25
1	A	205	LYS	CA-C-N	-5.62	117.42	122.43
1	A	205	LYS	C-N-CA	-5.62	117.42	122.43
1	B	207	ARG	CD-NE-CZ	5.62	132.27	124.40
1	A	79	GLU	CA-C-N	5.62	131.62	121.06
1	A	79	GLU	C-N-CA	5.62	131.62	121.06
1	D	276	VAL	CB-CA-C	5.62	124.28	111.02
1	A	77	PRO	O-C-N	-5.62	116.12	122.91
1	A	173	ASP	CB-CG-OD1	5.62	131.31	118.40
1	B	267	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	B	11	ALA	CA-C-N	-5.60	112.07	121.75
1	B	11	ALA	C-N-CA	-5.60	112.07	121.75
1	A	314	GLU	CA-C-O	-5.59	114.53	120.40
1	B	69	GLN	CA-C-O	-5.59	114.62	120.55
1	B	169	GLN	OE1-CD-NE2	-5.59	117.01	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	SER	N-CA-C	-5.59	103.15	110.53
1	B	234	ALA	N-CA-C	5.59	119.28	112.23
1	A	76	VAL	CA-C-N	5.59	125.90	119.92
1	A	76	VAL	C-N-CA	5.59	125.90	119.92
1	B	157	MET	CA-CB-CG	-5.59	102.92	114.10
1	B	226	ASP	N-CA-CB	5.59	118.11	110.01
1	C	248	GLY	CA-C-N	5.59	130.88	123.05
1	C	248	GLY	C-N-CA	5.59	130.88	123.05
1	D	274	ARG	CA-C-O	-5.59	114.79	120.71
1	B	258	LEU	CA-C-O	5.58	127.42	121.11
1	A	102	GLN	CG-CD-NE2	-5.58	108.03	116.40
1	B	41	ARG	CG-CD-NE	5.58	124.28	112.00
1	A	340	ASN	CB-CA-C	-5.58	101.73	110.94
1	B	76	VAL	O-C-N	-5.57	115.12	121.14
1	C	183	GLN	CA-C-O	5.57	126.44	120.70
1	A	378	CYS	CA-C-O	-5.57	114.52	120.92
1	C	313	VAL	CA-C-O	5.57	127.74	121.28
1	B	4	SER	CA-C-N	-5.57	115.85	123.14
1	B	4	SER	C-N-CA	-5.57	115.85	123.14
1	D	129	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	C	56	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	D	36	SER	CA-C-O	-5.56	112.54	119.38
1	A	220	ARG	CA-CB-CG	-5.56	102.99	114.10
1	C	227	SER	CA-C-N	5.55	127.72	120.28
1	C	227	SER	C-N-CA	5.55	127.72	120.28
1	A	313	VAL	CA-C-O	-5.55	114.96	120.90
1	A	181	ALA	CA-C-O	-5.54	113.84	120.10
1	B	122	ALA	CB-CA-C	5.54	118.11	109.42
1	D	14	ALA	N-CA-C	-5.54	102.69	110.50
1	B	56	GLN	O-C-N	-5.54	115.23	122.59
1	D	60	ALA	CA-C-O	5.53	126.98	120.96
1	A	178	PHE	CA-C-N	5.53	127.62	120.44
1	A	178	PHE	C-N-CA	5.53	127.62	120.44
1	B	17	SER	CA-C-N	5.53	130.04	121.26
1	B	17	SER	C-N-CA	5.53	130.04	121.26
1	B	369	GLY	CA-C-N	5.52	128.71	120.87
1	B	369	GLY	C-N-CA	5.52	128.71	120.87
1	C	302	ARG	NH1-CZ-NH2	5.52	126.48	119.30
1	A	249	LEU	O-C-N	-5.52	116.76	123.27
1	B	44	VAL	N-CA-CB	5.52	117.61	110.99
1	A	217	GLU	N-CA-C	5.51	119.85	113.18
1	B	388	CYS	O-C-N	-5.51	116.74	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	MET	O-C-N	5.51	129.32	123.42
1	B	232	ARG	CA-C-N	5.51	125.69	119.90
1	B	232	ARG	C-N-CA	5.51	125.69	119.90
1	A	8	ALA	N-CA-C	5.51	119.26	112.54
1	B	294	PRO	CA-C-N	5.51	128.11	120.29
1	B	294	PRO	C-N-CA	5.51	128.11	120.29
1	C	150	ASP	N-CA-CB	5.51	118.12	109.69
1	B	71	ALA	CA-C-N	5.50	127.97	120.54
1	B	71	ALA	C-N-CA	5.50	127.97	120.54
1	A	365	MET	O-C-N	-5.50	116.37	122.09
1	A	375	ALA	O-C-N	5.50	129.74	123.31
1	C	162	GLU	N-CA-CB	5.50	118.20	110.12
1	C	359	ASN	CB-CA-C	-5.49	102.26	110.88
1	A	355	ALA	CA-C-N	-5.49	112.92	120.28
1	A	355	ALA	C-N-CA	-5.49	112.92	120.28
1	A	367	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	B	91	SER	O-C-N	5.47	127.78	122.09
1	B	109	SER	CB-CA-C	-5.47	100.86	109.34
1	B	66	PRO	N-CD-CG	-5.47	95.00	103.20
1	A	200	VAL	CA-C-N	5.46	125.22	119.76
1	A	200	VAL	C-N-CA	5.46	125.22	119.76
1	B	227	SER	O-C-N	-5.46	115.30	122.39
1	B	332	TRP	CH2-CZ2-CE2	-5.46	110.40	117.50
1	D	138	LYS	CG-CD-CE	5.46	123.86	111.30
1	A	58	LEU	O-C-N	-5.46	116.46	121.37
1	A	191	LYS	CA-C-O	-5.45	114.77	120.55
1	A	353	SER	CA-C-O	-5.45	112.71	120.51
1	C	137	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	35	ILE	CB-CG1-CD1	5.45	125.25	113.80
1	C	21	ALA	O-C-N	-5.45	116.34	122.12
1	A	347	GLY	CA-C-O	5.45	126.98	122.13
1	A	300	LEU	CA-C-O	5.45	126.51	120.63
1	D	25	THR	CB-CA-C	-5.45	103.64	109.85
1	A	56	GLN	CA-C-O	5.44	128.29	120.51
1	A	346	ILE	CB-CG1-CD1	5.44	125.22	113.80
1	B	161	ALA	CA-C-N	5.44	127.51	120.44
1	B	161	ALA	C-N-CA	5.44	127.51	120.44
1	A	389	ILE	CA-C-N	-5.43	114.28	122.81
1	A	389	ILE	C-N-CA	-5.43	114.28	122.81
1	D	200	VAL	CG1-CB-CG2	-5.43	98.85	110.80
1	B	257	LEU	CD1-CG-CD2	-5.42	98.88	110.80
1	B	316	ASN	N-CA-C	5.42	117.94	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	GLY	N-CA-C	-5.42	107.60	114.16
1	C	65	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	300	LEU	O-C-N	-5.41	116.39	122.12
1	B	389	ILE	N-CA-CB	5.41	120.31	111.44
1	A	150	ASP	N-CA-C	-5.40	101.66	110.20
1	B	85	MET	CA-CB-CG	5.40	124.90	114.10
1	B	380	GLY	N-CA-C	-5.40	105.72	111.93
1	D	360	THR	O-C-N	-5.40	116.47	122.09
1	A	334	PRO	CB-CA-C	5.40	119.51	111.85
1	A	317	GLU	N-CA-C	5.39	117.70	109.62
1	B	189	ALA	N-CA-C	-5.39	105.32	111.14
1	C	264	ALA	N-CA-CB	5.38	117.96	109.94
1	D	53	ILE	CA-C-O	-5.38	114.56	120.48
1	A	136	ASP	CA-C-O	-5.38	115.75	121.94
1	D	385	VAL	N-CA-CB	5.38	119.38	111.52
1	A	253	ALA	N-CA-CB	5.38	120.65	111.66
1	B	372	LYS	CD-CE-NZ	-5.38	94.69	111.90
1	B	266	ARG	N-CA-CB	5.38	118.02	110.12
1	B	176	ASP	CA-C-O	5.37	126.25	120.55
1	A	316	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	B	348	HIS	CB-CA-C	-5.37	103.38	111.27
1	C	186	ALA	O-C-N	5.37	128.87	122.27
1	A	13	THR	O-C-N	-5.37	116.05	122.65
1	A	231	LEU	CB-CG-CD1	-5.36	94.61	110.70
1	D	358	LEU	CB-CA-C	-5.36	102.43	110.90
1	B	163	ASN	CB-CA-C	-5.36	101.90	110.79
1	B	86	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	B	356	ARG	N-CA-C	-5.36	105.36	111.14
1	A	298	LYS	CA-CB-CG	5.35	124.81	114.10
1	A	174	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	203	ILE	O-C-N	-5.35	115.91	122.97
1	B	313	VAL	CA-CB-CG1	5.35	119.49	110.40
1	A	305	TRP	CA-C-O	5.34	128.02	121.56
1	B	358	LEU	N-CA-C	-5.34	105.35	111.07
1	A	307	ILE	CA-C-N	5.34	133.09	121.19
1	A	307	ILE	C-N-CA	5.34	133.09	121.19
1	D	134	MET	O-C-N	-5.34	117.16	123.41
1	C	217	GLU	N-CA-C	5.34	119.64	113.18
1	A	242	THR	CA-C-O	-5.33	112.88	120.51
1	A	348	HIS	CA-C-N	5.33	126.51	119.84
1	A	348	HIS	C-N-CA	5.33	126.51	119.84
1	B	49	VAL	N-CA-CB	5.33	116.86	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ALA	CA-C-O	5.33	126.60	121.00
1	D	306	LYS	CA-C-O	-5.33	115.16	121.66
1	A	244	GLY	CA-C-O	5.33	126.87	120.90
1	A	302	ARG	N-CA-CB	-5.33	101.55	110.39
1	D	107	ASP	CB-CA-C	5.32	120.36	109.55
1	D	333	ASP	CA-C-O	5.32	124.76	119.49
1	B	198	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	56	GLN	CB-CG-CD	-5.32	103.55	112.60
1	D	109	SER	N-CA-CB	5.32	118.11	110.40
1	A	355	ALA	N-CA-C	-5.32	105.15	111.69
1	C	176	ASP	CA-C-O	5.32	126.18	120.70
1	C	245	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	B	276	VAL	CA-C-O	-5.31	113.47	119.42
1	A	245	ASN	CA-C-O	-5.31	113.01	119.43
1	C	117	GLU	CB-CA-C	-5.31	100.31	109.86
1	D	160	THR	N-CA-CB	5.30	118.39	110.22
1	B	220	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	B	139	MET	N-CA-C	-5.30	99.88	108.41
1	B	340	ASN	CB-CG-OD1	-5.30	110.20	120.80
1	B	156	HIS	N-CA-C	5.30	116.93	110.41
1	B	385	VAL	CA-C-N	5.30	131.03	122.29
1	B	385	VAL	C-N-CA	5.30	131.03	122.29
1	A	348	HIS	CB-CA-C	-5.29	103.50	111.27
1	B	67	ALA	CA-C-O	5.29	126.56	120.90
1	C	199	ILE	CB-CA-C	-5.29	104.28	111.15
1	B	231	LEU	CD1-CG-CD2	5.28	122.42	110.80
1	C	184	ASN	CB-CA-C	5.28	119.18	110.88
1	B	41	ARG	NH1-CZ-NH2	-5.28	112.43	119.30
1	B	298	LYS	N-CA-C	5.28	116.72	111.07
1	C	287	VAL	CA-C-O	5.28	127.38	120.78
1	A	232	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	267	ARG	CG-CD-NE	-5.28	100.39	112.00
1	B	85	MET	N-CA-C	-5.28	101.10	108.96
1	C	348	HIS	N-CA-C	5.27	117.52	108.82
1	A	53	ILE	CB-CG1-CD1	-5.27	102.74	113.80
1	A	162	GLU	CA-C-N	5.27	127.77	120.29
1	A	162	GLU	C-N-CA	5.27	127.77	120.29
1	A	298	LYS	CA-C-N	-5.26	113.60	120.44
1	A	298	LYS	C-N-CA	-5.26	113.60	120.44
1	A	145	LYS	N-CA-C	5.26	116.70	111.07
1	A	295	ALA	CA-C-O	-5.26	113.92	119.97
1	C	378	CYS	N-CA-CB	5.26	118.87	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	GLN	N-CA-CB	5.26	119.29	111.51
1	A	83	TRP	O-C-N	5.25	129.04	123.42
1	A	29	GLU	CA-C-N	5.25	127.75	120.29
1	A	29	GLU	C-N-CA	5.25	127.75	120.29
1	A	262	ALA	O-C-N	5.25	128.73	122.27
1	B	234	ALA	N-CA-CB	-5.25	102.21	110.30
1	A	314	GLU	CB-CG-CD	5.25	121.52	112.60
1	B	144	ILE	O-C-N	5.25	128.77	121.84
1	B	71	ALA	O-C-N	-5.25	116.67	122.07
1	A	110	ILE	CB-CG1-CD1	5.24	124.81	113.80
1	A	263	GLU	CB-CA-C	5.24	119.60	110.79
1	D	13	THR	N-CA-C	-5.24	102.24	110.36
1	A	360	THR	CA-C-O	5.24	126.10	120.55
1	C	318	ALA	O-C-N	-5.24	116.58	122.03
1	B	110	ILE	N-CA-C	5.23	115.52	107.77
1	A	50	ASN	O-C-N	5.23	129.97	122.28
1	D	119	MET	CG-SD-CE	5.23	112.41	100.90
1	A	169	GLN	N-CA-CB	-5.23	103.96	111.91
1	A	185	LYS	CA-C-O	-5.22	113.96	119.97
1	B	86	ASN	N-CA-C	5.22	116.70	107.61
1	B	120	SER	N-CA-CB	5.22	117.89	110.16
1	A	276	VAL	O-C-N	5.22	127.42	122.20
1	A	385	VAL	CA-C-O	5.22	126.48	120.90
1	A	195	PHE	CG-CD1-CE1	5.21	129.56	120.70
1	B	81	THR	CA-CB-CG2	5.21	119.36	110.50
1	B	378	CYS	CB-CA-C	5.21	118.13	109.53
1	C	96	VAL	CA-CB-CG1	5.21	119.25	110.40
1	B	381	GLY	CA-C-O	-5.21	113.24	119.07
1	C	16	GLY	O-C-N	-5.21	115.68	122.81
1	A	33	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	44	VAL	O-C-N	-5.20	117.72	123.18
1	A	122	ALA	N-CA-C	-5.20	103.23	109.83
1	C	161	ALA	CB-CA-C	-5.20	102.72	110.88
1	A	308	GLY	N-CA-C	-5.20	108.95	114.67
1	A	120	SER	CB-CA-C	-5.20	101.85	110.68
1	A	171	SER	CA-C-O	-5.19	115.97	121.94
1	A	172	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	274	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	A	301	GLU	CA-C-N	-5.19	112.05	120.72
1	A	301	GLU	C-N-CA	-5.19	112.05	120.72
1	A	391	SER	CB-CA-C	-5.19	100.75	109.83
1	C	107	ASP	CA-C-O	5.19	125.34	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	SER	CA-CB-OG	-5.19	100.72	111.10
1	B	172	ARG	N-CA-C	-5.19	104.69	111.02
1	B	101	GLN	CA-C-O	5.18	126.05	120.55
1	B	178	PHE	CD1-CE1-CZ	5.18	129.33	120.00
1	C	202	PHE	CA-C-O	-5.18	114.73	120.38
1	A	172	ARG	N-CA-CB	5.18	118.22	109.78
1	A	266	ARG	CD-NE-CZ	5.18	131.65	124.40
1	A	223	ALA	CA-C-O	5.18	126.82	120.92
1	B	11	ALA	CA-C-O	5.17	126.55	120.75
1	C	110	ILE	CB-CG1-CD1	5.17	124.67	113.80
1	C	310	LEU	CA-C-O	-5.17	115.02	120.92
1	C	247	SER	CA-CB-OG	-5.17	100.76	111.10
1	B	116	MET	N-CA-C	-5.17	100.88	108.79
1	C	241	VAL	CA-C-O	-5.17	115.04	120.57
1	A	92	GLY	N-CA-C	-5.16	106.54	112.73
1	B	177	ALA	N-CA-CB	5.16	117.70	110.12
1	B	368	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	274	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	C	255	ALA	CA-C-O	5.16	126.83	121.36
1	D	23	ALA	CB-CA-C	-5.15	100.18	110.42
1	B	300	LEU	CA-C-N	5.15	127.13	120.44
1	B	300	LEU	C-N-CA	5.15	127.13	120.44
1	C	267	ARG	CD-NE-CZ	5.14	131.60	124.40
1	A	337	VAL	CA-C-N	-5.14	115.06	122.36
1	A	337	VAL	C-N-CA	-5.14	115.06	122.36
1	B	39	LEU	N-CA-CB	-5.14	102.62	110.07
1	B	212	THR	O-C-N	5.14	129.08	123.27
1	C	233	PRO	CA-C-O	-5.14	115.17	121.03
1	D	13	THR	CB-CA-C	-5.14	100.47	111.78
1	B	13	THR	CB-CA-C	-5.14	99.53	109.76
1	C	360	THR	CA-C-N	5.14	127.48	120.54
1	C	360	THR	C-N-CA	5.14	127.48	120.54
1	B	267	ARG	CA-C-O	5.14	125.85	119.12
1	B	305	TRP	CE3-CZ3-CH2	5.13	127.78	121.10
1	B	259	MET	CA-C-O	-5.13	115.94	121.38
1	C	339	VAL	N-CA-CB	-5.13	103.56	110.54
1	A	348	HIS	N-CA-C	5.13	117.47	108.75
1	B	81	THR	O-C-N	-5.13	115.61	122.94
1	A	171	SER	N-CA-C	5.13	117.14	110.53
1	B	340	ASN	O-C-N	-5.13	115.95	122.26
1	D	68	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	C	266	ARG	CB-CA-C	-5.12	101.16	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	PRO	O-C-N	-5.11	116.50	122.99
1	D	338	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	210	ASP	CB-CG-OD1	5.11	130.14	118.40
1	A	16	GLY	O-C-N	-5.10	115.91	123.11
1	A	5	ILE	N-CA-CB	5.10	119.54	111.99
1	B	43	GLY	O-C-N	-5.10	115.99	122.32
1	B	258	LEU	N-CA-C	5.10	117.89	109.72
1	A	45	ALA	N-CA-C	5.10	117.44	110.55
1	A	232	ARG	CA-C-O	5.10	125.88	120.63
1	D	368	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	A	275	ILE	CB-CA-C	5.10	116.74	111.23
1	B	66	PRO	CA-C-O	-5.10	111.80	119.55
1	C	254	ALA	N-CA-CB	5.10	119.24	110.77
1	A	138	LYS	CA-C-O	5.09	126.86	121.05
1	A	266	ARG	N-CA-CB	5.09	117.61	110.12
1	A	392	LEU	N-CA-CB	5.09	119.16	110.50
1	C	266	ARG	N-CA-CB	5.09	118.07	110.22
1	C	302	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	A	65	ASN	N-CA-CB	-5.09	101.31	110.37
1	A	287	VAL	CA-CB-CG2	5.09	119.06	110.40
1	B	361	LEU	N-CA-C	5.09	116.52	111.07
1	B	269	ILE	CB-CG1-CD1	-5.09	103.11	113.80
1	D	219	ILE	CA-C-O	-5.09	115.76	121.36
1	D	142	THR	CA-CB-CG2	-5.09	101.85	110.50
1	D	299	ALA	CA-C-N	5.08	127.40	120.54
1	D	299	ALA	C-N-CA	5.08	127.40	120.54
1	A	155	TYR	CA-CB-CG	5.08	123.04	113.90
1	D	184	ASN	O-C-N	5.08	127.30	122.07
1	A	136	ASP	N-CA-CB	-5.08	103.18	110.44
1	A	183	GLN	CA-C-N	5.07	127.08	120.28
1	A	183	GLN	C-N-CA	5.07	127.08	120.28
1	B	46	ALA	O-C-N	-5.07	116.29	122.22
1	A	52	VAL	CA-C-O	-5.07	115.06	120.59
1	D	79	GLU	CB-CG-CD	5.07	121.21	112.60
1	C	29	GLU	CB-CG-CD	5.06	121.20	112.60
1	B	251	ASP	CA-C-O	5.06	126.48	120.66
1	B	314	GLU	CA-CB-CG	-5.06	103.98	114.10
1	D	52	VAL	CA-C-O	5.06	125.70	120.39
1	B	36	SER	N-CA-CB	5.06	117.64	110.16
1	A	332	TRP	O-C-N	-5.05	117.03	122.79
1	D	340	ASN	CA-C-O	-5.04	113.78	119.78
1	A	35	ILE	CB-CA-C	-5.04	105.33	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ALA	CB-CA-C	-5.04	102.97	110.88
1	D	76	VAL	CA-CB-CG2	-5.04	101.84	110.40
1	A	8	ALA	CA-C-N	5.04	132.13	121.91
1	A	8	ALA	C-N-CA	5.04	132.13	121.91
1	B	177	ALA	CA-C-N	5.04	126.99	120.44
1	B	177	ALA	C-N-CA	5.04	126.99	120.44
1	B	255	ALA	CA-C-O	5.04	126.72	121.38
1	A	22	PHE	O-C-N	-5.03	116.07	122.26
1	B	268	GLY	CA-C-N	-5.03	113.32	122.43
1	B	268	GLY	C-N-CA	-5.03	113.32	122.43
1	A	386	ALA	O-C-N	5.03	129.11	123.27
1	C	324	CYS	CA-CB-SG	-5.03	102.84	114.40
1	A	64	GLN	O-C-N	5.03	129.18	122.95
1	C	139	MET	CA-C-O	-5.02	115.08	120.46
1	B	14	ALA	N-CA-CB	5.02	117.42	110.04
1	D	240	THR	N-CA-CB	-5.02	104.35	110.98
1	D	88	LEU	CA-C-N	5.02	127.51	120.28
1	D	88	LEU	C-N-CA	5.02	127.51	120.28
1	A	197	ASP	CB-CG-OD2	5.02	129.94	118.40
1	B	128	LEU	N-CA-C	5.01	120.01	112.94
1	D	52	VAL	O-C-N	-5.01	117.85	123.26
1	A	79	GLU	CG-CD-OE2	5.01	129.92	118.40
1	A	323	ALA	N-CA-CB	5.01	117.27	110.01
1	B	235	PHE	CA-C-N	-5.01	116.00	123.11
1	B	235	PHE	C-N-CA	-5.01	116.00	123.11
1	C	336	ILE	CA-C-O	5.00	124.52	119.97
1	C	102	GLN	OE1-CD-NE2	5.00	127.60	122.60
1	D	37	ALA	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	VAL	Mainchain
1	A	203	ILE	Mainchain
1	A	315	ALA	Mainchain
1	B	358	LEU	Mainchain
1	B	51	GLU	Mainchain
1	B	93	LEU	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	2813	0	2819	94	0
1	B	2813	0	2819	82	0
1	C	2813	0	2819	98	0
1	D	2813	0	2819	96	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	8	0	14	7	0
3	B	8	0	14	12	0
3	C	8	0	14	15	0
3	D	8	0	14	20	0
4	A	293	0	0	16	0
4	B	287	0	0	17	0
4	C	101	0	0	7	0
4	D	70	0	0	14	0
All	All	12065	0	11332	385	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (385) 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)
3:D:1004:MPD:CM	3:D:1004:MPD:C2	1.79	1.59
3:B:1002:MPD:C2	3:B:1002:MPD:CM	1.79	1.58
3:A:1001:MPD:CM	3:A:1001:MPD:C2	1.79	1.58
3:C:1003:MPD:C2	3:C:1003:MPD:CM	1.81	1.57
3:C:1003:MPD:CM	3:C:1003:MPD:H4	1.67	1.24
3:C:1003:MPD:CM	3:C:1003:MPD:C4	2.15	1.23
1:A:258:LEU:HG	4:A:2051:HOH:O	1.40	1.22
3:D:1004:MPD:HM1	3:D:1004:MPD:H4	1.24	1.15
3:D:1004:MPD:CM	3:D:1004:MPD:H4	1.81	1.11
3:D:1004:MPD:CM	3:D:1004:MPD:C4	2.31	1.08
3:C:1003:MPD:CM	3:C:1003:MPD:C3	2.34	1.06
1:C:81:THR:HG22	1:D:383:MET:HG2	1.39	1.03
3:B:1002:MPD:CM	3:B:1002:MPD:C4	2.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1003:MPD:C4	3:C:1003:MPD:HM1	1.82	1.02
3:B:1002:MPD:CM	3:B:1002:MPD:H4	1.90	1.02
3:B:1002:MPD:CM	3:B:1002:MPD:C3	2.38	1.01
3:C:1003:MPD:H4	3:C:1003:MPD:HM1	1.03	1.01
1:C:64:GLN:HE22	1:D:157:MET:HE3	1.26	1.00
3:D:1004:MPD:CM	3:D:1004:MPD:C3	2.40	1.00
1:C:156:HIS:HE1	3:C:1003:MPD:HM3	1.28	0.96
3:B:1002:MPD:H4	3:B:1002:MPD:HM1	1.48	0.93
1:C:156:HIS:CE1	3:C:1003:MPD:HM3	2.03	0.92
3:A:1001:MPD:CM	3:A:1001:MPD:C3	2.48	0.91
1:B:4:SER:N	4:B:2282:HOH:O	2.04	0.90
1:D:156:HIS:HE1	3:D:1004:MPD:HM3	1.38	0.88
1:D:290:THR:HA	4:D:1056:HOH:O	1.74	0.87
1:C:203:ILE:HD13	1:C:212:THR:HG23	1.59	0.84
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.44	0.82
1:D:156:HIS:CE1	3:D:1004:MPD:HM3	2.15	0.82
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.46	0.80
1:B:258:LEU:HG	4:B:2222:HOH:O	1.82	0.80
1:A:156:HIS:HB2	4:A:2232:HOH:O	1.82	0.80
1:B:156:HIS:CE1	3:B:1002:MPD:HM3	2.17	0.80
1:B:316:ASN:HB3	4:B:2027:HOH:O	1.81	0.80
3:C:1003:MPD:C4	3:C:1003:MPD:HM2	2.11	0.79
1:C:57:VAL:HG12	1:C:58:LEU:HG	1.64	0.78
3:B:1002:MPD:C4	3:B:1002:MPD:HM2	2.12	0.77
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.20	0.75
1:D:96:VAL:HG12	1:D:387:MET:HE1	1.66	0.75
1:B:156:HIS:HE1	3:B:1002:MPD:HM3	1.50	0.75
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.68	0.74
1:C:64:GLN:NE2	1:D:157:MET:HE3	2.00	0.74
1:C:168:TRP:CH2	1:C:329:ASP:HB2	2.25	0.72
1:A:206:GLY:HA3	1:A:209:GLY:O	1.88	0.72
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.02	0.71
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.54	0.71
1:A:228:MET:HE1	1:A:244:GLY:C	2.16	0.71
1:D:263:GLU:OE1	1:D:266:ARG:NH1	2.24	0.71
1:C:292:PRO:HB3	1:C:376:THR:OG1	1.91	0.70
1:D:317:GLU:HB3	1:D:344:ILE:HG13	1.74	0.70
1:C:268:GLY:HA2	4:C:1094:HOH:O	1.89	0.70
1:A:88:LEU:HD12	1:A:380:GLY:O	1.93	0.69
1:C:300:LEU:HD13	1:C:307:ILE:HG12	1.75	0.69
1:A:387:MET:SD	4:A:2167:HOH:O	2.51	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ALA:HB1	1:D:269:ILE:HG21	1.74	0.67
1:A:298:LYS:NZ	1:A:298:LYS:HA	2.09	0.67
3:D:1004:MPD:C4	3:D:1004:MPD:HM2	2.23	0.67
1:A:371:ARG:HG3	4:A:2211:HOH:O	1.95	0.67
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.76	0.67
3:D:1004:MPD:HM1	3:D:1004:MPD:C4	2.05	0.67
1:B:171:SER:OG	4:B:2186:HOH:O	2.12	0.67
1:A:225:LEU:HG	4:A:2205:HOH:O	1.94	0.66
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.60	0.66
1:C:361:LEU:O	1:C:365:MET:HG3	1.96	0.66
1:A:387:MET:HE3	1:A:389:ILE:HD11	1.77	0.65
1:A:228:MET:HE3	4:A:2123:HOH:O	1.96	0.64
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.32	0.64
1:B:356:ARG:C	1:B:356:ARG:HD2	2.22	0.64
1:B:98:LEU:O	1:B:102:GLN:HG2	1.97	0.64
1:B:296:SER:HB3	1:B:374:LEU:HD11	1.78	0.64
1:C:171:SER:OG	4:C:1027:HOH:O	2.15	0.64
1:B:228:MET:HE2	4:B:2023:HOH:O	1.96	0.64
1:C:139:MET:CE	1:D:139:MET:HE1	2.28	0.64
1:B:5:ILE:HD12	1:B:103:ILE:CG2	2.28	0.63
1:C:133:LYS:HG2	4:C:1074:HOH:O	1.98	0.63
3:C:1003:MPD:HM2	3:C:1003:MPD:O4	1.96	0.63
1:B:191:LYS:NZ	1:B:191:LYS:HB3	2.13	0.63
1:D:72:MET:HE1	1:D:78:GLN:HB3	1.80	0.63
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.63	0.63
1:C:293:ILE:HB	1:C:294:PRO:HD3	1.80	0.63
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.63	0.63
1:A:280:THR:HG23	1:B:81:THR:HG21	1.80	0.63
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.14	0.63
1:D:258:LEU:HD22	1:D:258:LEU:N	2.14	0.62
1:B:156:HIS:HE1	3:B:1002:MPD:CM	2.12	0.62
1:A:176:ASP:O	1:A:180:VAL:HG23	2.00	0.62
1:D:27:ALA:HB1	1:D:116:MET:HB2	1.82	0.62
1:C:148:LEU:HD22	3:C:1003:MPD:HM2	1.82	0.61
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.18	0.61
1:C:207:ARG:HG2	1:C:207:ARG:HH11	1.63	0.61
1:A:298:LYS:O	1:A:298:LYS:HD3	2.01	0.61
1:A:133:LYS:HA	4:A:2258:HOH:O	2.01	0.61
1:B:187:GLU:HG2	4:B:2220:HOH:O	2.00	0.61
1:C:322:GLN:O	1:C:326:VAL:HG23	2.01	0.60
1:C:348:HIS:HD2	3:C:1003:MPD:H53	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:HA3	1:A:111:ILE:HG21	1.82	0.60
1:B:5:ILE:HD12	1:B:103:ILE:HG22	1.83	0.60
3:D:1004:MPD:O4	4:D:1042:HOH:O	2.10	0.60
1:D:97:ALA:O	1:D:101:GLN:HG3	2.01	0.59
1:C:269:ILE:O	1:C:271:PRO:HD3	2.01	0.59
1:C:12:ARG:HB2	1:C:254:ALA:HB2	1.84	0.59
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.37	0.59
1:D:156:HIS:HE1	3:D:1004:MPD:CM	2.12	0.59
1:D:180:VAL:HG22	1:D:228:MET:HE3	1.85	0.59
1:A:9:SER:HA	1:A:272:LEU:HD22	1.85	0.59
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.15	0.58
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.84	0.58
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.16	0.58
1:C:379:ILE:HG21	1:C:383:MET:HE3	1.86	0.57
1:C:311:ASP:HB2	1:C:370:ALA:HB1	1.86	0.57
1:B:134:MET:HE2	1:C:144:ILE:HD11	1.87	0.57
1:C:247:SER:OG	1:C:348:HIS:HB2	2.04	0.57
1:C:28:HIS:HB2	1:C:70:ALA:HB2	1.87	0.57
1:A:162:GLU:OE2	4:A:2240:HOH:O	2.17	0.57
1:A:298:LYS:HD3	1:A:298:LYS:C	2.30	0.56
1:B:9:SER:HA	1:B:272:LEU:HD22	1.87	0.56
1:A:168:TRP:O	1:A:169:GLN:HB2	2.04	0.56
1:B:156:HIS:ND1	1:B:157:MET:N	2.53	0.56
1:A:236:ASP:O	1:A:237:LYS:C	2.49	0.56
1:B:174:GLU:HB3	4:B:2186:HOH:O	2.06	0.56
1:C:105:THR:OG1	1:C:107:ASP:OD2	2.22	0.56
1:A:316:ASN:HB3	4:A:2204:HOH:O	2.06	0.56
1:C:292:PRO:HD3	1:C:378:CYS:HB3	1.87	0.56
1:B:361:LEU:O	1:B:365:MET:HG3	2.06	0.55
1:C:361:LEU:HD13	1:C:365:MET:SD	2.47	0.55
1:C:300:LEU:CD1	1:C:307:ILE:HG12	2.35	0.55
1:A:12:ARG:O	1:A:199:ILE:HA	2.07	0.55
3:A:1001:MPD:CM	3:A:1001:MPD:O2	2.52	0.55
1:B:41:ARG:HD2	4:B:2190:HOH:O	2.06	0.54
1:C:364:GLU:O	1:C:368:ARG:HG2	2.06	0.54
1:B:191:LYS:HB3	1:B:191:LYS:HZ1	1.72	0.54
1:A:366:LYS:NZ	4:A:2094:HOH:O	2.40	0.54
1:B:158:GLY:O	1:B:161:ALA:HB3	2.08	0.54
1:B:232:ARG:O	4:B:2131:HOH:O	2.18	0.54
1:C:156:HIS:HE1	3:C:1003:MPD:CM	2.11	0.54
1:C:158:GLY:O	1:C:161:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HA	1:A:298:LYS:HZ3	1.71	0.54
1:D:53:ILE:HD13	1:D:83:TRP:CZ2	2.42	0.54
1:B:38:VAL:HA	4:B:2190:HOH:O	2.07	0.54
1:D:298:LYS:HE2	1:D:302:ARG:HG3	1.88	0.54
1:B:41:ARG:CD	4:B:2190:HOH:O	2.56	0.53
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.23	0.53
1:C:280:THR:HG23	1:D:81:THR:HG21	1.90	0.53
1:A:116:MET:HA	1:A:253:ALA:HA	1.89	0.53
1:D:99:GLY:O	1:D:103:ILE:HD12	2.08	0.53
1:D:206:GLY:HA3	1:D:209:GLY:O	2.08	0.53
1:C:239:GLY:HA3	4:C:1100:HOH:O	2.08	0.53
1:D:174:GLU:OE2	1:D:328:LYS:NZ	2.41	0.53
3:B:1002:MPD:H4	3:B:1002:MPD:HM2	1.80	0.52
1:D:5:ILE:HD12	1:D:103:ILE:CG2	2.39	0.52
3:D:1004:MPD:H51	4:D:1073:HOH:O	2.08	0.52
1:A:7:ILE:HG12	1:A:258:LEU:CD1	2.40	0.52
1:A:236:ASP:OD1	1:A:238:GLU:N	2.36	0.52
1:A:354:GLY:HA2	1:A:377:LEU:HD21	1.92	0.52
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.44	0.52
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.92	0.52
1:A:186:ALA:HB2	1:A:341:GLY:HA3	1.92	0.52
1:B:37:ALA:HB2	1:B:200:VAL:HG21	1.91	0.52
1:A:156:HIS:HE1	3:A:1001:MPD:HM2	1.75	0.52
1:C:53:ILE:HD13	1:C:83:TRP:CZ2	2.45	0.51
1:B:134:MET:HE3	1:C:143:MET:HE1	1.92	0.51
1:C:279:ALA:CB	1:C:298:LYS:HB3	2.40	0.51
1:D:99:GLY:HA3	4:D:1030:HOH:O	2.09	0.51
1:A:85:MET:HA	1:B:85:MET:HA	1.92	0.51
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.75	0.51
1:D:148:LEU:HD22	3:D:1004:MPD:HM2	1.91	0.51
1:D:249:LEU:HD23	3:D:1004:MPD:H11	1.92	0.51
1:B:51:GLU:OE2	1:B:81:THR:OG1	2.25	0.51
1:D:207:ARG:N	1:D:207:ARG:HD3	2.25	0.51
1:D:278:TRP:HA	1:D:386:ALA:O	2.10	0.51
3:C:1003:MPD:CM	3:C:1003:MPD:C1	2.78	0.51
1:B:258:LEU:N	1:B:258:LEU:HD22	2.26	0.51
1:D:119:MET:HE3	1:D:350:ILE:CD1	2.41	0.51
1:B:171:SER:HB2	4:B:2266:HOH:O	2.10	0.51
1:A:358:LEU:HD11	1:A:387:MET:HE1	1.92	0.50
1:A:181:ALA:O	1:A:185:LYS:HG3	2.11	0.50
1:A:236:ASP:O	1:A:238:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:OD1	1:A:236:ASP:C	2.53	0.50
1:D:258:LEU:HD23	4:D:1030:HOH:O	2.10	0.50
1:C:139:MET:HE1	1:D:139:MET:HE1	1.93	0.50
1:A:93:LEU:HD11	1:A:387:MET:HE2	1.93	0.50
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.92	0.50
1:D:266:ARG:NH2	4:D:1051:HOH:O	2.44	0.50
1:B:64:GLN:O	1:B:65:ASN:C	2.55	0.50
1:D:77:PRO:HA	4:D:1008:HOH:O	2.12	0.50
1:A:340:ASN:HB2	4:A:2047:HOH:O	2.12	0.50
1:B:186:ALA:HA	1:B:340:ASN:O	2.11	0.50
1:B:298:LYS:HE3	1:B:298:LYS:HA	1.93	0.50
1:C:213:VAL:HA	4:C:1098:HOH:O	2.10	0.50
1:B:274:ARG:HD2	4:B:2282:HOH:O	2.12	0.50
1:D:5:ILE:HD12	1:D:103:ILE:HG22	1.93	0.50
1:D:50:ASN:O	1:D:80:ALA:HB1	2.12	0.50
1:A:200:VAL:O	1:A:200:VAL:HG13	2.11	0.50
1:B:136:ASP:OD1	1:C:140:ILE:HA	2.12	0.50
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.73	0.49
1:A:162:GLU:O	1:A:166:LYS:HG3	2.12	0.49
1:B:156:HIS:HB2	4:B:2287:HOH:O	2.13	0.49
1:B:28:HIS:ND1	1:B:62:GLU:OE2	2.28	0.49
1:D:275:ILE:HA	1:D:389:ILE:HD13	1.94	0.49
1:B:181:ALA:O	1:B:185:LYS:HG3	2.12	0.49
1:B:191:LYS:HG3	4:B:2220:HOH:O	2.13	0.49
1:C:293:ILE:HB	1:C:294:PRO:CD	2.43	0.49
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.38	0.49
1:D:313:VAL:HG12	1:D:337:VAL:HG13	1.95	0.49
1:B:392:LEU:HD12	4:B:2137:HOH:O	2.12	0.49
1:D:357:ILE:CD1	1:D:375:ALA:HB1	2.43	0.49
1:C:54:LEU:CD1	1:C:116:MET:HE2	2.43	0.48
1:A:207:ARG:HG2	1:A:208:LYS:H	1.77	0.48
1:B:100:MET:C	1:B:100:MET:HE2	2.38	0.48
1:C:257:LEU:HD22	1:C:259:MET:HE3	1.95	0.48
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.48	0.48
1:D:156:HIS:ND1	1:D:157:MET:N	2.61	0.48
1:D:247:SER:OG	3:D:1004:MPD:H53	2.13	0.48
1:A:220:ARG:NH2	4:A:2097:HOH:O	2.46	0.48
1:C:112:VAL:HG12	1:C:113:ALA:N	2.28	0.48
1:A:158:GLY:O	1:A:161:ALA:HB3	2.13	0.48
1:B:372:LYS:HE3	4:B:2211:HOH:O	2.12	0.48
1:B:257:LEU:HD23	1:B:257:LEU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ILE:HG23	1:D:387:MET:SD	2.54	0.48
1:C:186:ALA:HA	1:C:340:ASN:O	2.14	0.48
1:C:139:MET:SD	1:D:139:MET:HE1	2.54	0.47
1:C:385:VAL:HG22	1:C:386:ALA:N	2.29	0.47
1:D:101:GLN:O	1:D:105:THR:HG23	2.14	0.47
3:D:1004:MPD:HM2	3:D:1004:MPD:O4	2.13	0.47
1:A:58:LEU:HB3	4:A:2225:HOH:O	2.15	0.47
1:A:105:THR:HG21	1:B:101:GLN:HG2	1.97	0.47
1:C:155:TYR:CD2	1:C:159:THR:HG21	2.49	0.47
1:C:170:LEU:HD13	1:C:324:CYS:HB2	1.96	0.47
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.96	0.47
1:D:322:GLN:O	1:D:326:VAL:HG23	2.15	0.47
1:D:333:ASP:OD1	1:D:335:SER:OG	2.31	0.47
1:B:132:VAL:O	1:D:129:ARG:HA	2.14	0.47
1:C:110:ILE:HD13	1:C:259:MET:HE2	1.97	0.47
1:D:348:HIS:CD2	3:D:1004:MPD:H53	2.49	0.47
1:A:191:LYS:NZ	4:A:2217:HOH:O	2.48	0.47
1:A:196:LYS:NZ	4:A:2224:HOH:O	2.47	0.47
1:C:207:ARG:HD3	1:C:207:ARG:N	2.29	0.47
1:C:129:ARG:HD3	1:D:18:PHE:CZ	2.50	0.47
1:D:64:GLN:O	1:D:65:ASN:C	2.58	0.47
1:A:279:ALA:HB1	1:A:298:LYS:HG3	1.95	0.47
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.67	0.46
3:C:1003:MPD:CM	3:C:1003:MPD:O2	2.56	0.46
1:A:37:ALA:HB2	1:A:200:VAL:HG21	1.96	0.46
1:D:272:LEU:HD21	4:D:1040:HOH:O	2.15	0.46
1:A:124:HIS:HA	1:A:140:ILE:O	2.15	0.46
1:A:293:ILE:HB	1:A:294:PRO:CD	2.46	0.46
1:D:35:ILE:O	1:D:38:VAL:HG22	2.16	0.46
1:A:249:LEU:HD21	3:A:1001:MPD:C1	2.46	0.46
1:A:337:VAL:O	1:A:338:ASN:C	2.59	0.46
1:A:389:ILE:HG22	1:A:390:GLU:N	2.30	0.46
1:C:195:PHE:O	1:C:198:GLU:HG2	2.16	0.46
1:D:190:GLN:NE2	1:D:219:ILE:HD12	2.31	0.46
1:A:319:PHE:CE1	3:A:1001:MPD:HM1	2.52	0.45
1:A:361:LEU:O	1:A:365:MET:HG3	2.16	0.45
1:B:350:ILE:HD13	1:B:350:ILE:HG21	1.82	0.45
1:B:94:ARG:O	1:B:97:ALA:HB3	2.17	0.45
1:C:157:MET:O	1:C:158:GLY:C	2.60	0.45
1:C:187:GLU:OE2	1:C:221:HIS:HA	2.17	0.45
1:D:51:GLU:HB3	1:D:111:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:OE1	1:A:344:ILE:HG13	2.17	0.45
1:C:7:ILE:HG21	1:C:362:LEU:CD1	2.47	0.45
1:C:85:MET:HA	1:D:85:MET:HA	1.99	0.45
1:D:298:LYS:HE2	1:D:302:ARG:CG	2.47	0.45
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.82	0.45
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.50	0.45
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.51	0.45
1:D:364:GLU:O	1:D:368:ARG:HG2	2.17	0.45
1:C:57:VAL:HB	1:C:117:GLU:OE1	2.17	0.44
1:B:348:HIS:CD2	3:B:1002:MPD:H53	2.52	0.44
1:D:46:ALA:HB3	4:D:1064:HOH:O	2.17	0.44
3:D:1004:MPD:CM	3:D:1004:MPD:O2	2.55	0.44
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.48	0.44
1:B:263:GLU:OE1	1:B:266:ARG:NH2	2.51	0.44
1:A:196:LYS:O	1:A:196:LYS:HG2	2.16	0.44
1:A:305:TRP:CE2	1:A:372:LYS:HD3	2.53	0.44
1:C:7:ILE:HG21	1:C:362:LEU:HD13	1.98	0.44
1:D:305:TRP:CZ3	1:D:372:LYS:HB3	2.52	0.44
1:D:357:ILE:HD12	1:D:375:ALA:HB1	2.00	0.44
1:C:362:LEU:CD2	1:C:389:ILE:HG21	2.46	0.44
1:A:12:ARG:HD2	1:A:356:ARG:HG2	2.00	0.44
1:A:350:ILE:HD13	1:A:350:ILE:HG21	1.53	0.44
1:B:356:ARG:HD2	1:B:356:ARG:O	2.17	0.44
1:D:316:ASN:ND2	1:D:348:HIS:CE1	2.86	0.44
1:D:317:GLU:O	1:D:343:ALA:HB3	2.18	0.44
1:A:293:ILE:HG23	1:A:329:ASP:OD1	2.17	0.44
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.85	0.44
1:B:359:ASN:O	1:B:360:THR:C	2.57	0.44
1:B:124:HIS:HA	1:B:140:ILE:O	2.18	0.43
1:C:54:LEU:O	1:C:84:GLY:HA2	2.18	0.43
1:D:12:ARG:HB2	1:D:254:ALA:HB2	2.01	0.43
1:D:39:LEU:HB3	1:D:44:VAL:O	2.18	0.43
1:C:293:ILE:CB	1:C:294:PRO:HD3	2.46	0.43
1:B:124:HIS:HB3	1:B:139:MET:HE3	2.00	0.43
3:B:1002:MPD:HM2	3:B:1002:MPD:O4	2.18	0.43
1:C:329:ASP:C	1:C:329:ASP:OD1	2.61	0.43
1:C:57:VAL:CG2	1:C:88:LEU:HA	2.49	0.43
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.54	0.43
1:B:313:VAL:HB	1:B:337:VAL:HG22	1.99	0.43
1:A:183:GLN:HA	1:A:345:ALA:HB2	2.01	0.43
1:C:266:ARG:NH2	4:C:1053:HOH:O	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ILE:CG2	1:C:383:MET:HE3	2.49	0.43
1:A:225:LEU:O	1:A:228:MET:HB2	2.18	0.43
1:B:263:GLU:O	1:B:264:ALA:C	2.61	0.43
1:D:25:THR:HA	1:D:26:PRO:HD3	1.87	0.43
1:A:133:LYS:O	1:A:134:MET:HB2	2.19	0.42
1:B:57:VAL:HG21	1:B:350:ILE:HG22	2.01	0.42
1:C:157:MET:HE2	1:C:157:MET:HA	2.01	0.42
1:C:288:MET:HG3	4:C:1009:HOH:O	2.19	0.42
1:D:263:GLU:O	1:D:264:ALA:C	2.61	0.42
1:B:5:ILE:HG13	1:B:100:MET:HG2	2.01	0.42
1:A:260:SER:HB2	4:A:2135:HOH:O	2.19	0.42
1:A:31:GLY:O	1:A:35:ILE:HG13	2.19	0.42
1:B:175:GLN:NE2	1:B:240:THR:HG23	2.33	0.42
1:D:186:ALA:HA	1:D:340:ASN:O	2.20	0.42
1:D:249:LEU:CD2	3:D:1004:MPD:H11	2.49	0.42
1:A:52:VAL:O	1:A:82:ALA:HA	2.18	0.42
1:B:136:ASP:HA	1:C:139:MET:O	2.19	0.42
1:B:257:LEU:HD23	1:B:258:LEU:N	2.34	0.42
1:C:103:ILE:HA	1:C:108:ALA:O	2.19	0.42
1:C:226:ASP:O	1:C:230:LYS:HG3	2.19	0.42
1:C:358:LEU:O	1:C:362:LEU:HG	2.19	0.42
1:D:143:MET:HE1	1:D:249:LEU:HD13	2.01	0.42
1:A:53:ILE:HD13	1:A:53:ILE:HG21	1.89	0.42
1:A:96:VAL:HG11	1:A:387:MET:HE1	2.01	0.42
1:C:156:HIS:ND1	1:C:157:MET:N	2.67	0.42
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.78	0.42
1:C:284:ASP:OD2	1:C:286:LYS:NZ	2.49	0.42
1:A:258:LEU:N	1:A:258:LEU:HD22	2.34	0.42
1:B:349:PRO:O	1:B:350:ILE:C	2.63	0.42
1:B:88:LEU:HD12	1:B:380:GLY:O	2.20	0.42
1:C:297:ARG:HG2	1:C:297:ARG:NH1	2.33	0.42
1:D:28:HIS:HA	1:D:116:MET:SD	2.60	0.42
1:A:99:GLY:CA	1:A:111:ILE:HG21	2.48	0.41
1:A:361:LEU:HD22	1:A:365:MET:HG3	2.01	0.41
1:B:293:ILE:HB	1:B:294:PRO:CD	2.50	0.41
1:C:17:SER:HB2	1:C:217:GLU:OE2	2.19	0.41
1:C:155:TYR:CG	1:C:159:THR:HG21	2.55	0.41
1:C:279:ALA:HB3	1:C:298:LYS:HB3	2.02	0.41
1:C:186:ALA:HB2	1:C:341:GLY:HA3	2.01	0.41
1:D:111:ILE:HB	4:D:1030:HOH:O	2.20	0.41
1:D:172:ARG:NH1	4:D:1046:HOH:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.85	0.41
1:A:280:THR:HA	1:A:384:GLY:O	2.20	0.41
1:D:56:GLN:HB3	4:D:1019:HOH:O	2.20	0.41
1:A:207:ARG:HH11	1:A:207:ARG:CG	2.34	0.41
1:A:264:ALA:O	1:A:265:SER:C	2.63	0.41
1:B:374:LEU:HD23	1:B:374:LEU:C	2.45	0.41
1:C:162:GLU:OE1	1:C:240:THR:HG22	2.20	0.41
1:C:343:ALA:O	1:C:344:ILE:C	2.63	0.41
1:D:89:CYS:HB3	4:D:1031:HOH:O	2.20	0.41
1:D:293:ILE:HB	1:D:294:PRO:HD3	2.02	0.41
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.86	0.41
1:C:305:TRP:NE1	1:C:372:LYS:NZ	2.69	0.41
1:A:298:LYS:HA	1:A:298:LYS:HZ2	1.81	0.41
1:B:8:ALA:HA	1:B:271:PRO:HB3	2.02	0.41
1:C:293:ILE:CB	1:C:294:PRO:CD	2.99	0.41
1:A:249:LEU:CD2	3:A:1001:MPD:H12	2.51	0.41
1:A:292:PRO:HD3	1:A:378:CYS:HA	2.01	0.41
1:B:207:ARG:HG2	1:B:208:LYS:H	1.85	0.41
1:D:183:GLN:CD	1:D:220:ARG:HG2	2.44	0.41
3:D:1004:MPD:CM	3:D:1004:MPD:C1	2.81	0.41
1:A:51:GLU:OE2	1:A:81:THR:OG1	2.36	0.41
1:A:168:TRP:CZ3	1:A:328:LYS:HB3	2.56	0.41
1:B:139:MET:O	1:C:136:ASP:HA	2.21	0.41
1:B:236:ASP:O	1:B:237:LYS:C	2.62	0.41
1:D:312:LEU:O	1:D:373:GLY:HA2	2.21	0.41
1:A:77:PRO:HB2	1:A:79:GLU:OE1	2.21	0.41
1:A:133:LYS:H	1:A:133:LYS:HG2	1.42	0.41
1:B:57:VAL:HG21	1:B:350:ILE:CG2	2.50	0.41
1:D:312:LEU:HD13	1:D:368:ARG:HD2	2.02	0.41
1:B:236:ASP:O	1:B:238:GLU:N	2.54	0.40
1:C:350:ILE:HD13	1:C:350:ILE:HG21	1.86	0.40
1:B:274:ARG:NH2	1:B:390:GLU:OE1	2.55	0.40
1:D:46:ALA:N	4:D:1064:HOH:O	2.54	0.40
1:D:119:MET:HE3	1:D:350:ILE:HG13	2.02	0.40
1:A:191:LYS:HB3	1:A:191:LYS:HE2	1.94	0.40
1:C:18:PHE:O	1:C:19:ASN:C	2.64	0.40
1:D:265:SER:O	1:D:266:ARG:C	2.64	0.40
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.70	0.40
1:D:41:ARG:NH1	1:D:197:ASP:O	2.53	0.40
1:D:54:LEU:O	1:D:84:GLY:HA2	2.22	0.40
1:C:305:TRP:NE1	1:C:372:LYS:HZ3	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ASP:HB3	1:C:372:LYS:HD2	2.04	0.40
1:D:175:GLN:HB3	1:D:320:ALA:HB3	2.04	0.40
1:D:277:SER:OG	1:D:303:ALA:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	387/389 (100%)	363 (94%)	23 (6%)	1 (0%)	36	40
1	B	387/389 (100%)	366 (95%)	19 (5%)	2 (0%)	24	24
1	C	387/389 (100%)	364 (94%)	21 (5%)	2 (0%)	24	24
1	D	387/389 (100%)	367 (95%)	18 (5%)	2 (0%)	24	24
All	All	1548/1556 (100%)	1460 (94%)	81 (5%)	7 (0%)	24	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ILE
1	C	350	ILE
1	D	350	ILE
1	B	237	LYS
1	D	65	ASN
1	C	65	ASN
1	A	350	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	276/276 (100%)	248 (90%)	28 (10%)	7	5
1	B	276/276 (100%)	250 (91%)	26 (9%)	8	6
1	C	276/276 (100%)	249 (90%)	27 (10%)	7	5
1	D	276/276 (100%)	250 (91%)	26 (9%)	8	6
All	All	1104/1104 (100%)	997 (90%)	107 (10%)	8	6

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	5	ILE
1	A	39	LEU
1	A	59	PRO
1	A	124	HIS
1	A	198	GLU
1	A	207	ARG
1	A	225	LEU
1	A	230	LYS
1	A	232	ARG
1	A	237	LYS
1	A	240	THR
1	A	258	LEU
1	A	263	GLU
1	A	265	SER
1	A	272	LEU
1	A	276	VAL
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	339	VAL
1	A	350	ILE
1	A	353	SER
1	A	358	LEU
1	A	361	LEU
1	A	367	ARG
1	A	392	LEU

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Mol	Chain	Res	Type
1	B	38	VAL
1	B	39	LEU
1	B	133	LYS
1	B	134	MET
1	B	174	GLU
1	B	187	GLU
1	B	207	ARG
1	B	232	ARG
1	B	240	THR
1	B	257	LEU
1	B	258	LEU
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	276	VAL
1	B	296	SER
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	339	VAL
1	B	356	ARG
1	B	358	LEU
1	B	361	LEU
1	B	366	LYS
1	B	371	ARG
1	B	374	LEU
1	C	39	LEU
1	C	40	GLU
1	C	57	VAL
1	C	58	LEU
1	C	59	PRO
1	C	109	SER
1	C	110	ILE
1	C	134	MET
1	C	207	ARG
1	C	220	ARG
1	C	224	THR
1	C	237	LYS
1	C	258	LEU
1	C	272	LEU
1	C	276	VAL
1	C	297	ARG

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Mol	Chain	Res	Type
1	C	298	LYS
1	C	307	ILE
1	C	322	GLN
1	C	332	TRP
1	C	335	SER
1	C	339	VAL
1	C	353	SER
1	C	358	LEU
1	C	361	LEU
1	C	371	ARG
1	C	374	LEU
1	D	4	SER
1	D	30	LEU
1	D	34	VAL
1	D	36	SER
1	D	39	LEU
1	D	53	ILE
1	D	59	PRO
1	D	85	MET
1	D	144	ILE
1	D	187	GLU
1	D	192	ASP
1	D	204	VAL
1	D	207	ARG
1	D	224	THR
1	D	240	THR
1	D	249	LEU
1	D	258	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	335	SER
1	D	358	LEU
1	D	361	LEU
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	B	64	GLN
1	B	167	GLN
1	B	175	GLN
1	B	184	ASN
1	C	78	GLN
1	C	102	GLN
1	C	175	GLN
1	C	184	ASN
1	C	316	ASN
1	D	101	GLN
1	D	175	GLN
1	D	184	ASN
1	D	190	GLN
1	D	316	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	2005	-	4,4,4	0.96	0	6,6,6	1.11	0
2	SO4	B	2006	-	4,4,4	0.78	0	6,6,6	0.80	0
2	SO4	B	2001	-	4,4,4	0.80	0	6,6,6	0.43	0
3	MPD	A	1001	-	7,7,7	3.57	1 (14%)	9,10,10	2.91	5 (55%)
2	SO4	A	2002	-	4,4,4	0.74	0	6,6,6	0.63	0
2	SO4	A	2004	-	4,4,4	0.72	0	6,6,6	0.60	0
2	SO4	B	2003	-	4,4,4	0.67	0	6,6,6	0.71	0
3	MPD	C	1003	-	7,7,7	3.75	1 (14%)	9,10,10	2.38	3 (33%)
3	MPD	D	1004	-	7,7,7	3.59	1 (14%)	9,10,10	1.94	2 (22%)
3	MPD	B	1002	-	7,7,7	3.53	1 (14%)	9,10,10	2.30	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	1001	-	-	1/5/5/5	-
3	MPD	D	1004	-	-	3/5/5/5	-
3	MPD	B	1002	-	-	3/5/5/5	-
3	MPD	C	1003	-	-	3/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	MPD	CM-C2	9.77	1.81	1.52
3	D	1004	MPD	CM-C2	9.34	1.79	1.52
3	A	1001	MPD	CM-C2	9.17	1.79	1.52
3	B	1002	MPD	CM-C2	9.13	1.79	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	MPD	CM-C2-C3	-4.97	88.76	110.20
3	A	1001	MPD	O4-C4-C3	4.77	130.34	111.35
3	B	1002	MPD	CM-C2-C3	-4.42	91.14	110.20
3	A	1001	MPD	CM-C2-C1	4.31	120.27	110.63
3	B	1002	MPD	CM-C2-C1	4.22	120.07	110.63
3	D	1004	MPD	CM-C2-C3	-4.05	92.70	110.20
3	C	1003	MPD	C1-C2-C3	3.59	125.67	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1004	MPD	CM-C2-C1	3.10	117.57	110.63
3	A	1001	MPD	O2-C2-C1	-3.06	98.45	107.99
3	A	1001	MPD	CM-C2-C3	-2.97	97.40	110.20
3	A	1001	MPD	O2-C2-C3	2.72	119.43	109.27
3	B	1002	MPD	C5-C4-C3	-2.47	100.22	111.67
3	C	1003	MPD	CM-C2-C1	2.08	115.28	110.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1002	MPD	O2-C2-C3-C4
3	B	1002	MPD	CM-C2-C3-C4
3	C	1003	MPD	O2-C2-C3-C4
3	C	1003	MPD	CM-C2-C3-C4
3	D	1004	MPD	O2-C2-C3-C4
3	D	1004	MPD	CM-C2-C3-C4
3	A	1001	MPD	O2-C2-C3-C4
3	C	1003	MPD	C1-C2-C3-C4
3	D	1004	MPD	C1-C2-C3-C4
3	B	1002	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	MPD	7	0
3	C	1003	MPD	15	0
3	D	1004	MPD	20	0
3	B	1002	MPD	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/389 (100%)	-1.41	0 100 100	12, 22, 51, 92	0
1	B	389/389 (100%)	-1.37	0 100 100	14, 23, 50, 108	0
1	C	389/389 (100%)	-0.91	0 100 100	30, 52, 84, 122	0
1	D	389/389 (100%)	-0.78	0 100 100	30, 58, 109, 138	0
All	All	1556/1556 (100%)	-1.12	0 100 100	12, 44, 86, 138	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	D	1004	8/8	0.97	0.07	60,61,64,64	0
2	SO4	B	2001	5/5	0.98	0.05	74,75,76,76	0
3	MPD	A	1001	8/8	0.98	0.06	44,45,47,51	0
3	MPD	C	1003	8/8	0.98	0.07	56,57,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	2005	5/5	0.98	0.06	52,53,55,57	0
2	SO4	B	2006	5/5	0.99	0.04	39,41,45,45	0
2	SO4	A	2002	5/5	0.99	0.04	54,56,56,57	0
3	MPD	B	1002	8/8	0.99	0.04	36,38,39,39	0
2	SO4	A	2004	5/5	0.99	0.04	61,63,64,65	0
2	SO4	B	2003	5/5	0.99	0.04	55,56,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.