



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 07:52 am BST

PDB ID : 1E1C / pdb_00001e1c
Title : METHYLMALONYL-COA MUTASE H244A Mutant
Authors : Evans, P.R.; Thoma, N.H.
Deposited on : 2000-04-30
Resolution : 2.62 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

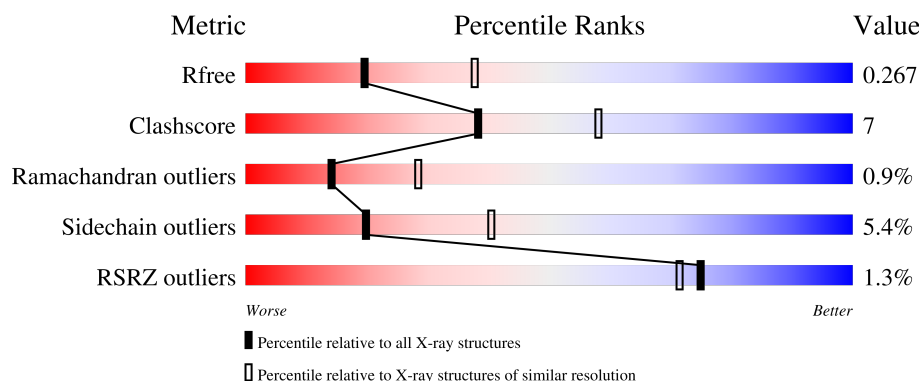
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	727	
1	C	727	
2	B	637	
2	D	637	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22307 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 METHYLMALONYL-COA MUTASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5558	3511	958	1065	24			
1	C	727	Total	C	N	O	S	0	0	0
			5558	3511	958	1065	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	HIS	engineered mutation	UNP P11652
C	244	ALA	HIS	engineered mutation	UNP P11652

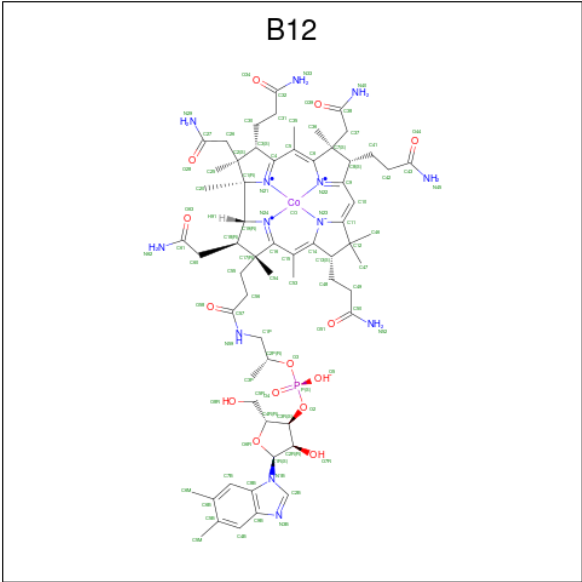
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			
2	D	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			

There are 6 discrepancies between the modelled and reference sequences:

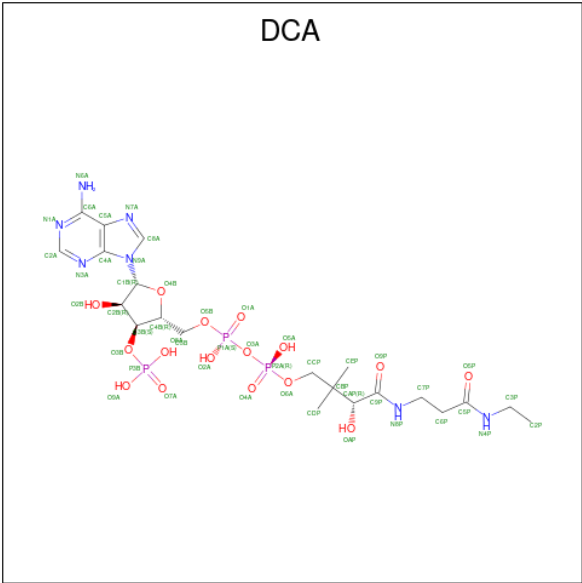
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is DESULFO-COENZYME A (CCD ID: DCA) (formula: $C_{21}H_{36}N_7O_{16}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			47	21	7	16	3		
4	C	1	Total	C	N	O	P	0	0
			47	21	7	16	3		

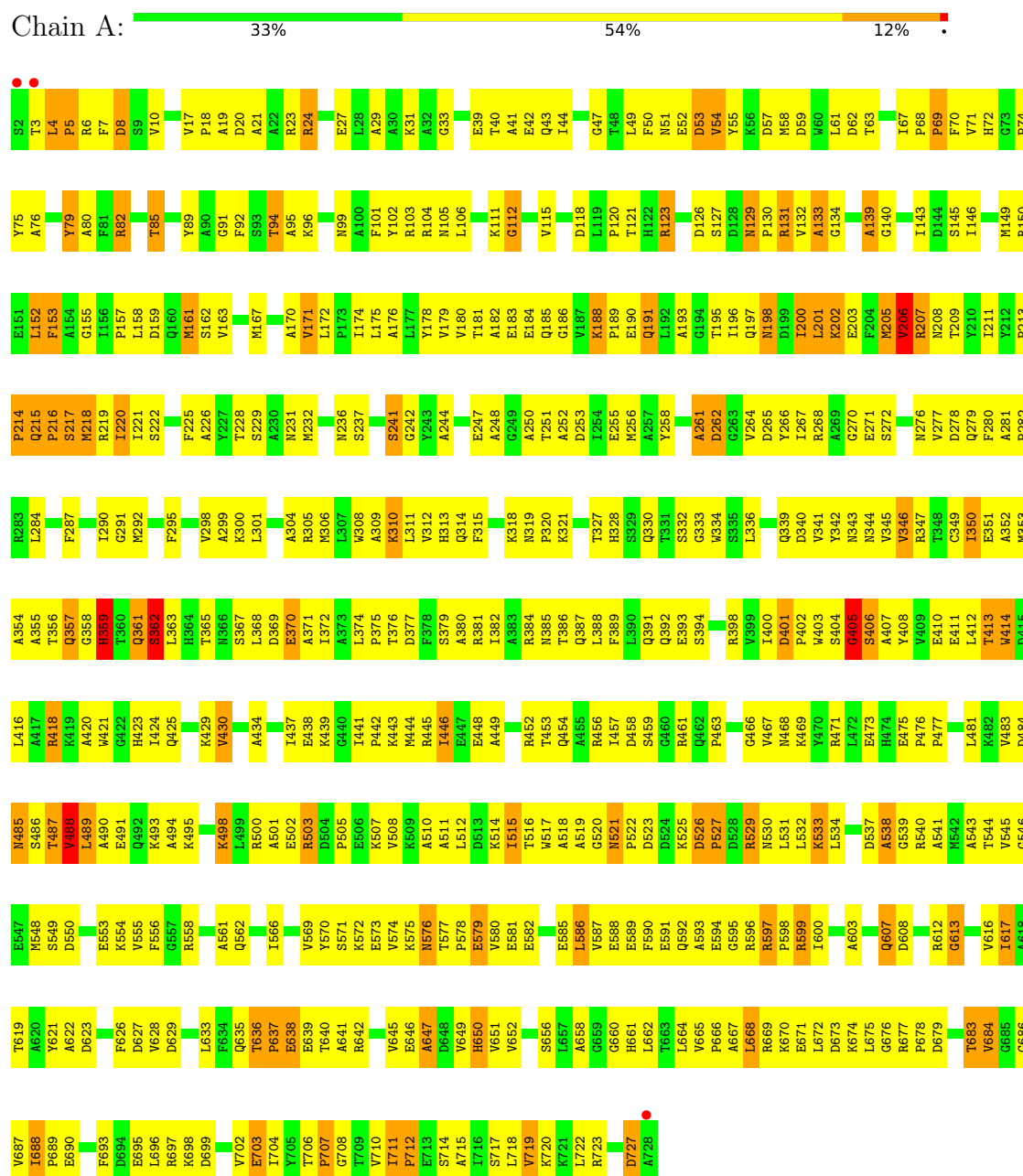
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	454	Total 454	O 454	0	0
5	B	316	Total 316	O 316	0	0
5	C	490	Total 490	O 490	0	0
5	D	265	Total 265	O 265	0	0

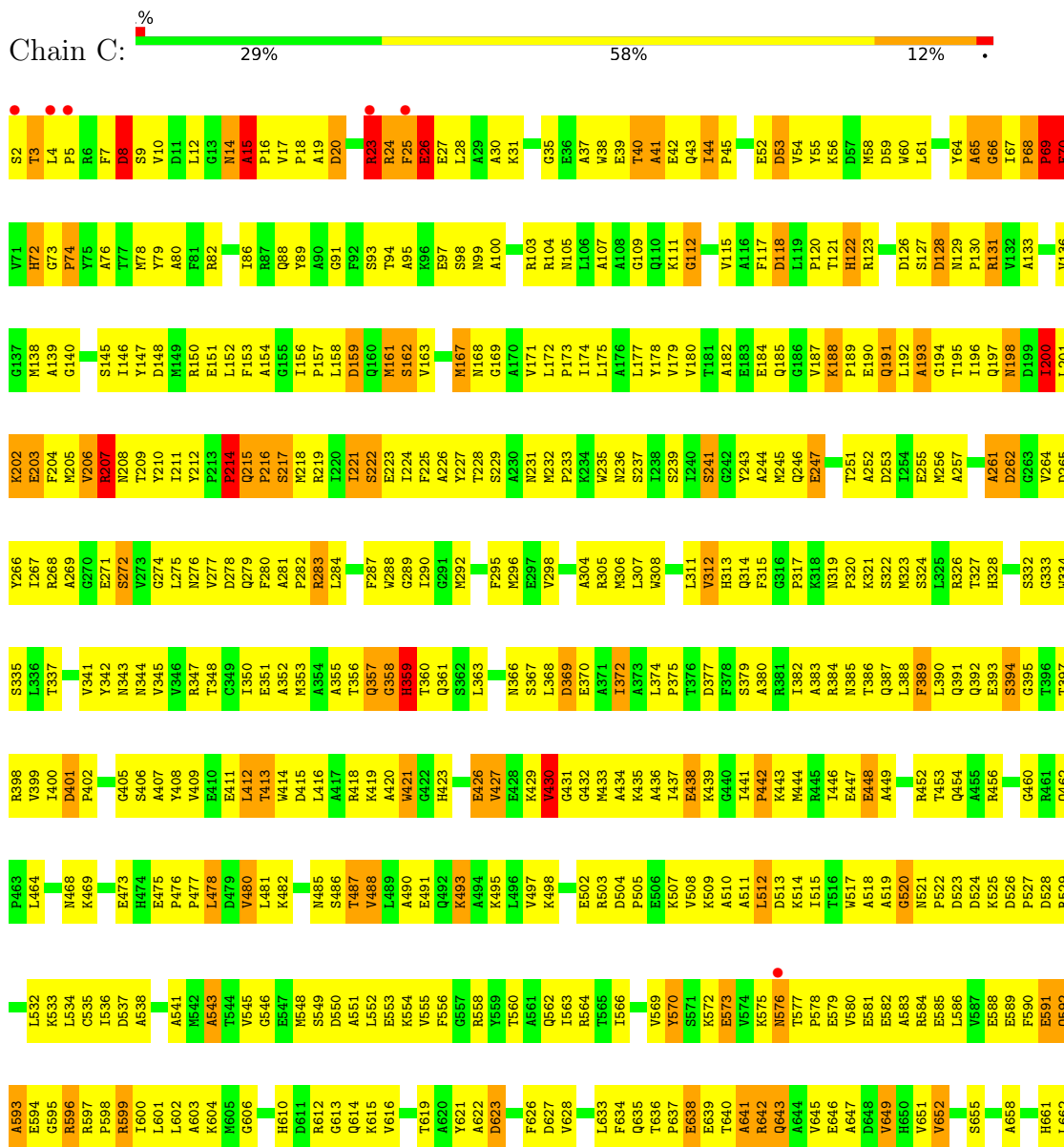
3 Residue-property plots

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.

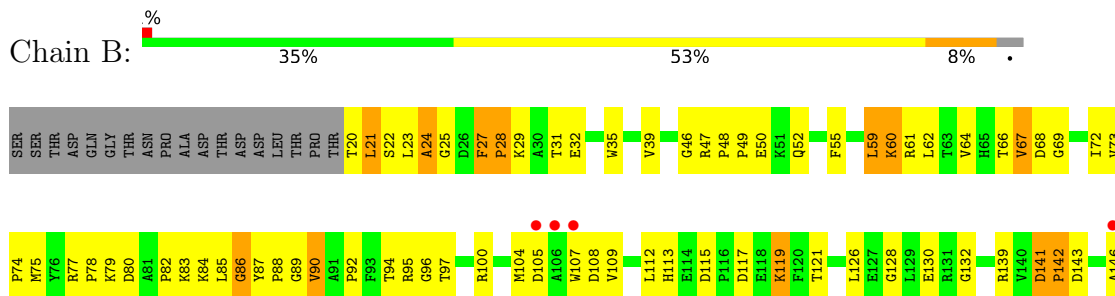
• Molecule 1: METHYLMALONYL-COA MUTASE ALPHA CHAIN

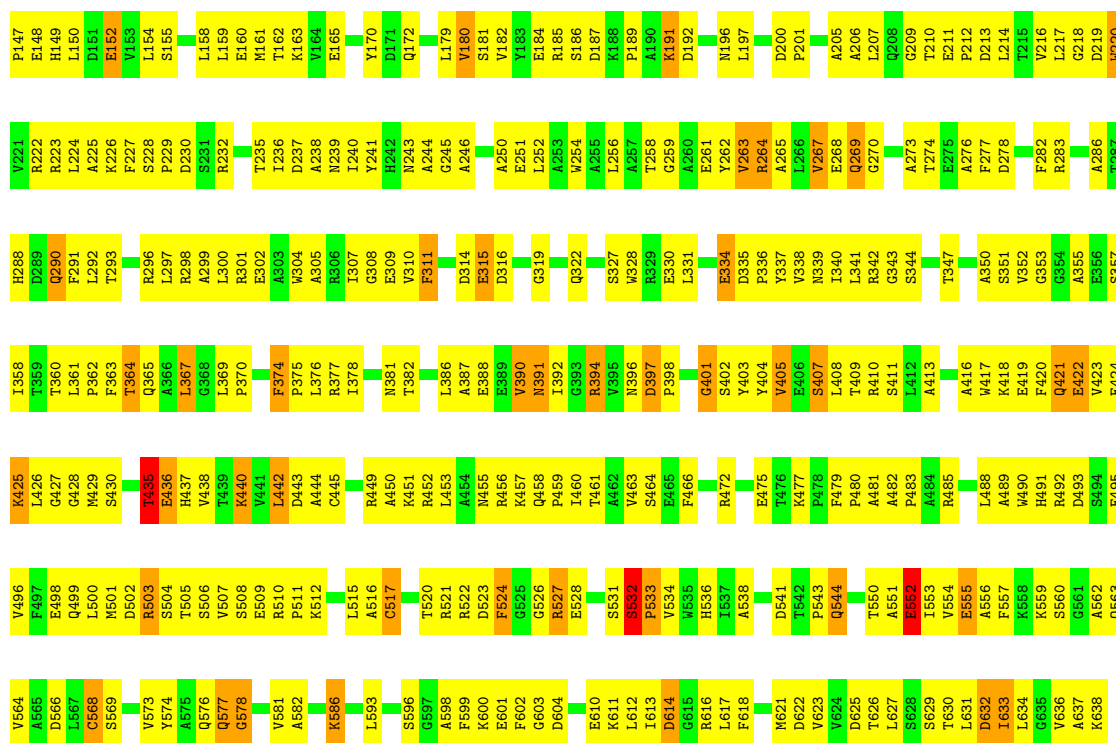


● Molecule 1: METHYLMALONYL-COA MUTASE ALPHA CHAIN

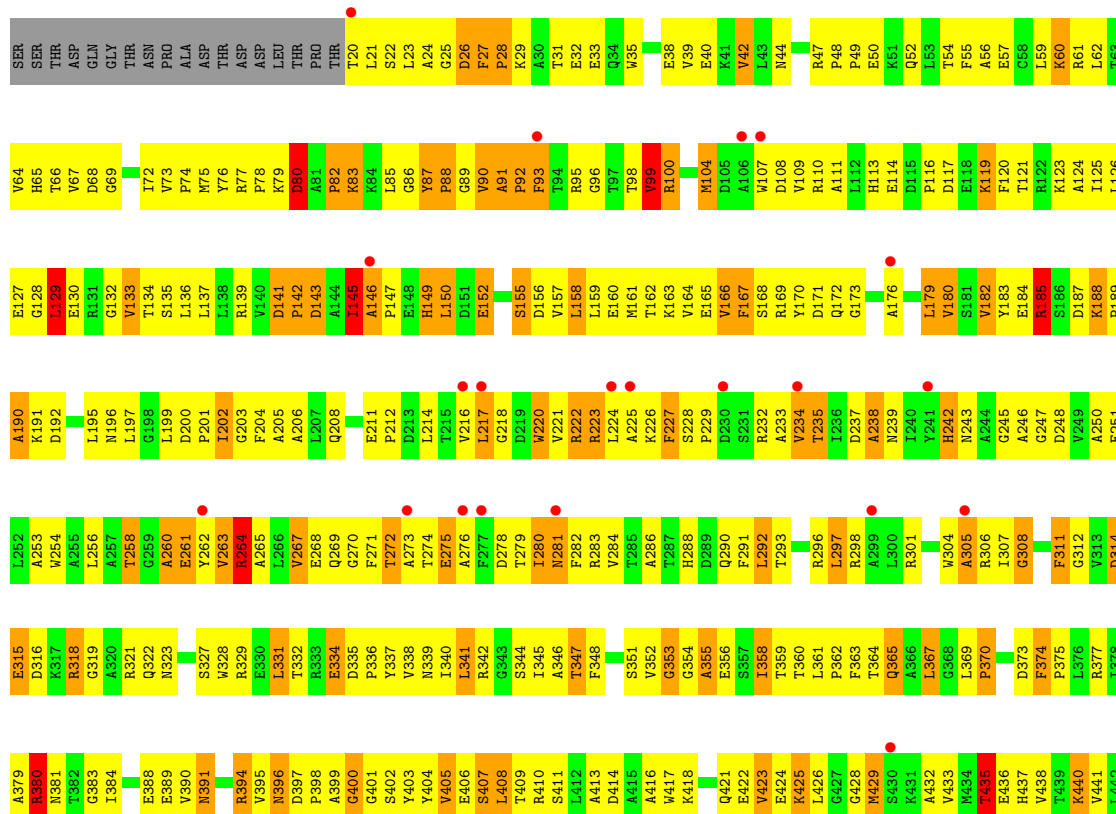


- Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN





• Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN



A582	K583	A584	L585	K586	A587	A588	G589	A590	L593	Y594	A598	F599	K600	E601	F602	D605	A606	A607	E608	A609	E610	K611	L612	I613	D614	G615	R616	L617	M621	D622	L627	S628	S629	T630	L631	D632	I633	L634	G635	V636	A637	K638											
F514	L515	A516	C517	I518	R521	R522	D523	F524	R527	E528	S531	S532	P533	V534	W535	H536	I537	I540	D541	T542	P543	Q544	V545	E546	G547	G548	T549	T550	A551	E552	I553	V554	E555	K558	K559	S560	G561	A562	A565	D566	L567	S570	A571	K572	V573	Y574	A575	Q576	Q577	E580	V581		
D443	A444	C445	N446	A447	E448	R449	A450	N455	R456	K457	Q458	P459	I460	T461	A462	V463	F466	P467	M468	I469	G470	A471	R472	S473	I474	E475	T476	K477	R478	F479	P480	A481	A482	P483	G487	L488	A489	W490	H491	R492	D493	S494	E495	E498	Q499	L500	M501	D502	V507	R510	P511	K512	V513

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.40Å 161.83Å 166.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 2.62 29.20 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.20-2.62) 97.4 (29.20-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.283 0.201 , 0.267	Depositor DCC
R_{free} test set	5001 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22307	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7263e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B12, DCA

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	1.10	6/5673 (0.1%)	3.34	925/7710 (12.0%)
1	C	1.09	7/5673 (0.1%)	3.33	975/7710 (12.6%)
2	B	1.04	6/4785 (0.1%)	3.27	746/6499 (11.5%)
2	D	0.97	5/4785 (0.1%)	3.29	782/6499 (12.0%)
All	All	1.06	24/20916 (0.1%)	3.31	3428/28418 (12.1%)

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	1
1	C	0	1
2	B	0	1
All	All	0	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	87	TYR	CA-CB	10.18	1.68	1.53
2	D	466	PHE	CA-CB	9.16	1.60	1.52
2	B	466	PHE	CA-CB	8.78	1.60	1.52
1	C	593	ALA	N-CA	-8.52	1.36	1.46
2	B	397	ASP	C-O	7.72	1.27	1.23
2	B	87	TYR	CA-CB	7.22	1.64	1.54
1	A	485	ASN	CA-CB	-6.97	1.42	1.53
1	C	42	GLU	N-CA	-6.40	1.37	1.46
2	B	270	GLY	N-CA	-5.86	1.36	1.45
2	B	458	GLN	N-CA	-5.72	1.39	1.46
1	C	593	ALA	C-N	-5.69	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	ILE	N-CA	-5.67	1.41	1.46
1	A	668	LEU	N-CA	-5.64	1.39	1.46
1	C	593	ALA	C-O	5.60	1.30	1.24
1	C	521	ASN	CA-CB	5.44	1.59	1.53
2	B	68	ASP	N-CA	-5.41	1.40	1.46
1	A	679	ASP	N-CA	-5.40	1.39	1.46
1	A	42	GLU	N-CA	-5.34	1.39	1.46
1	A	44	ILE	N-CA	-5.34	1.42	1.46
1	C	237	SER	C-N	-5.31	1.28	1.33
2	D	458	GLN	N-CA	-5.29	1.41	1.46
2	D	531	SER	CA-C	-5.26	1.46	1.52
2	D	90	VAL	N-CA	-5.19	1.39	1.46
1	C	315	PHE	N-CA	-5.17	1.39	1.46

All (3428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CA-CB-CG	47.27	159.87	112.60
2	B	61	ARG	CD-NE-CZ	33.00	170.60	124.40
1	C	485	ASN	CA-CB-CG	29.43	142.03	112.60
1	C	131	ARG	CD-NE-CZ	23.95	157.93	124.40
1	A	642	ARG	CD-NE-CZ	23.91	157.87	124.40
2	B	77	ARG	CD-NE-CZ	23.59	157.42	124.40
1	A	384	ARG	CD-NE-CZ	23.22	156.91	124.40
2	D	457	LYS	CA-C-N	22.44	143.24	122.37
2	D	457	LYS	C-N-CA	22.44	143.24	122.37
1	C	384	ARG	CD-NE-CZ	20.97	153.75	124.40
2	B	397	ASP	O-C-N	-19.17	112.71	121.53
2	D	187	ASP	CA-CB-CG	18.87	131.47	112.60
1	A	103	ARG	CD-NE-CZ	18.28	150.00	124.40
1	C	642	ARG	CD-NE-CZ	18.17	149.84	124.40
1	C	333	GLY	CA-C-O	17.76	139.48	120.66
1	A	638	GLU	CB-CG-CD	17.74	142.76	112.60
1	A	727	ASP	CA-CB-CG	17.71	130.31	112.60
2	B	187	ASP	CA-CB-CG	17.68	130.28	112.60
1	A	485	ASN	OD1-CG-ND2	17.21	139.81	122.60
1	C	576	ASN	CA-CB-CG	16.79	129.39	112.60
1	C	589	GLU	CB-CG-CD	16.56	140.75	112.60
2	B	225	ALA	CA-C-N	16.34	143.49	120.29
2	B	225	ALA	C-N-CA	16.34	143.49	120.29
2	B	269	GLN	CA-C-N	16.16	149.99	121.07
2	B	269	GLN	C-N-CA	16.16	149.99	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	LYS	CA-C-N	16.11	146.37	120.60
2	D	600	LYS	C-N-CA	16.11	146.37	120.60
1	C	133	ALA	CA-C-N	16.02	140.57	120.22
1	C	133	ALA	C-N-CA	16.02	140.57	120.22
2	B	239	ASN	CA-C-N	15.31	139.85	120.56
2	B	239	ASN	C-N-CA	15.31	139.85	120.56
1	C	513	ASP	CA-CB-CG	15.24	127.84	112.60
1	C	485	ASN	N-CA-CB	15.04	131.82	110.01
2	D	510	ARG	NE-CZ-NH2	14.91	132.62	119.20
1	C	41	ALA	O-C-N	-14.85	105.28	122.20
1	C	41	ALA	CA-C-N	14.68	150.25	121.18
1	C	41	ALA	C-N-CA	14.68	150.25	121.18
1	C	8	ASP	CA-C-N	14.46	144.94	122.24
1	C	8	ASP	C-N-CA	14.46	144.94	122.24
2	B	531	SER	N-CA-C	14.06	126.68	111.36
1	A	576	ASN	CA-CB-CG	14.05	126.65	112.60
1	A	678	PRO	CA-C-N	13.99	144.51	120.58
1	A	678	PRO	C-N-CA	13.99	144.51	120.58
1	A	556	PHE	CA-CB-CG	13.96	127.76	113.80
1	C	469	LYS	O-C-N	-13.95	107.09	123.41
2	D	352	VAL	CA-C-N	13.88	135.35	119.94
2	D	352	VAL	C-N-CA	13.88	135.35	119.94
2	D	223	ARG	CD-NE-CZ	13.48	143.27	124.40
2	D	311	PHE	CA-CB-CG	13.45	127.25	113.80
1	C	123	ARG	CD-NE-CZ	13.40	143.17	124.40
2	D	229	PRO	CA-C-N	13.38	139.29	120.29
2	D	229	PRO	C-N-CA	13.38	139.29	120.29
2	D	373	ASP	CA-CB-CG	13.35	125.95	112.60
1	C	727	ASP	CA-CB-CG	13.34	125.94	112.60
2	D	278	ASP	CA-C-O	-13.31	102.33	119.10
2	B	316	ASP	CA-CB-CG	13.30	125.90	112.60
1	A	41	ALA	CA-C-N	13.29	147.48	121.18
1	A	41	ALA	C-N-CA	13.29	147.48	121.18
1	C	117	PHE	CA-CB-CG	13.22	127.02	113.80
1	C	693	PHE	N-CA-C	13.22	127.16	111.82
1	A	569	VAL	N-CA-C	-13.18	100.22	111.56
1	A	622	ALA	O-C-N	-13.08	108.59	122.07
2	D	218	GLY	CA-C-N	13.01	138.77	120.29
2	D	218	GLY	C-N-CA	13.01	138.77	120.29
1	A	79	TYR	CA-C-N	13.01	137.71	120.28
1	A	79	TYR	C-N-CA	13.01	137.71	120.28
1	A	589	GLU	CB-CG-CD	12.97	134.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	VAL	CA-C-N	12.97	143.81	122.66
2	B	67	VAL	C-N-CA	12.97	143.81	122.66
2	B	229	PRO	CA-C-N	12.97	142.73	120.68
2	B	229	PRO	C-N-CA	12.97	142.73	120.68
1	C	314	GLN	CA-C-N	12.88	146.69	121.58
1	C	314	GLN	C-N-CA	12.88	146.69	121.58
1	C	343	ASN	CA-C-N	12.85	137.50	120.28
1	C	343	ASN	C-N-CA	12.85	137.50	120.28
2	B	531	SER	CA-C-O	12.84	134.03	120.42
2	D	172	GLN	CA-C-N	12.84	134.19	119.94
2	D	172	GLN	C-N-CA	12.84	134.19	119.94
1	C	17	VAL	N-CA-CB	12.63	126.22	111.31
1	C	633	LEU	CA-C-O	12.57	136.40	121.94
1	C	298	VAL	O-C-N	-12.55	109.39	121.94
2	B	72	ILE	CB-CG1-CD1	12.54	140.13	113.80
1	A	82	ARG	CD-NE-CZ	12.53	141.94	124.40
2	D	232	ARG	CA-CB-CG	12.52	139.15	114.10
1	A	52	GLU	CA-C-N	12.48	138.01	120.29
1	A	52	GLU	C-N-CA	12.48	138.01	120.29
2	D	48	PRO	N-CA-CB	12.46	110.17	103.19
1	A	131	ARG	CD-NE-CZ	12.46	141.84	124.40
2	D	77	ARG	CD-NE-CZ	12.38	141.74	124.40
2	D	306	ARG	CA-C-O	-12.36	108.02	121.00
2	B	430	SER	CA-C-N	12.36	137.25	120.44
2	B	430	SER	C-N-CA	12.36	137.25	120.44
1	A	313	HIS	CA-C-N	12.36	137.84	120.29
1	A	313	HIS	C-N-CA	12.36	137.84	120.29
1	A	485	ASN	N-CA-CB	12.31	128.21	110.12
2	B	47	ARG	CD-NE-CZ	12.29	141.60	124.40
2	B	243	ASN	CA-C-N	12.25	144.85	122.06
2	B	243	ASN	C-N-CA	12.25	144.85	122.06
1	A	41	ALA	O-C-N	-12.25	107.89	122.22
2	D	347	THR	O-C-N	-12.21	109.39	122.09
1	A	665	VAL	O-C-N	-12.19	112.62	120.42
2	D	150	LEU	CA-C-N	12.16	137.04	120.38
2	D	150	LEU	C-N-CA	12.16	137.04	120.38
2	D	600	LYS	O-C-N	-12.16	106.42	122.59
1	A	623	ASP	CA-CB-CG	12.11	124.71	112.60
2	D	239	ASN	CA-C-N	12.11	137.04	120.46
2	D	239	ASN	C-N-CA	12.11	137.04	120.46
1	A	526	ASP	CA-C-O	12.10	131.00	119.62
1	A	429	LYS	CA-C-N	12.08	141.65	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	LYS	C-N-CA	12.08	141.65	122.56
2	B	52	GLN	OE1-CD-NE2	12.05	134.65	122.60
1	C	520	GLY	O-C-N	-12.02	109.50	122.24
1	C	678	PRO	CA-C-O	11.97	132.33	118.68
1	A	185	GLN	CA-C-N	11.95	138.13	122.00
1	A	185	GLN	C-N-CA	11.95	138.13	122.00
2	D	96	GLY	CA-C-O	11.88	132.12	121.66
1	A	207	ARG	N-CA-C	11.85	127.93	113.23
2	D	238	ALA	CA-C-N	11.78	137.58	120.38
2	D	238	ALA	C-N-CA	11.78	137.58	120.38
2	D	490	TRP	O-C-N	-11.77	109.50	123.27
1	C	253	ASP	CA-CB-CG	11.77	124.37	112.60
2	D	192	ASP	CA-CB-CG	-11.76	100.84	112.60
1	C	430	VAL	O-C-N	-11.73	107.91	122.57
1	C	17	VAL	CA-C-O	11.71	128.15	119.25
2	D	314	ASP	CA-CB-CG	11.68	124.28	112.60
1	C	420	ALA	O-C-N	-11.62	110.11	122.07
1	C	596	ARG	NE-CZ-NH2	-11.58	108.78	119.20
2	B	105	ASP	CA-C-N	11.55	140.00	120.71
2	B	105	ASP	C-N-CA	11.55	140.00	120.71
1	C	622	ALA	N-CA-C	-11.51	98.26	111.03
2	D	305	ALA	CA-C-N	11.48	135.81	120.65
2	D	305	ALA	C-N-CA	11.48	135.81	120.65
1	C	670	LYS	CA-CB-CG	-11.47	91.16	114.10
2	B	577	GLN	OE1-CD-NE2	11.45	134.05	122.60
1	A	27	GLU	CA-C-N	11.42	135.29	120.44
1	A	27	GLU	C-N-CA	11.42	135.29	120.44
1	A	597	ARG	CD-NE-CZ	11.40	140.36	124.40
2	D	531	SER	N-CA-C	11.40	123.39	110.97
1	C	439	LYS	CA-C-N	11.40	141.27	120.87
1	C	439	LYS	C-N-CA	11.40	141.27	120.87
1	C	714	SER	CA-C-N	11.37	135.89	120.54
1	C	714	SER	C-N-CA	11.37	135.89	120.54
1	A	306	MET	CA-C-O	-11.37	108.89	120.82
2	B	67	VAL	O-C-N	-11.36	110.43	121.90
2	D	243	ASN	CA-C-N	11.35	141.89	122.26
2	D	243	ASN	C-N-CA	11.35	141.89	122.26
1	C	25	PHE	N-CA-C	-11.31	98.48	111.03
1	C	634	PHE	CA-CB-CG	11.30	125.10	113.80
2	D	327	SER	CA-C-O	11.30	133.80	120.92
1	C	438	GLU	CB-CG-CD	11.24	131.71	112.60
2	D	261	GLU	CA-C-N	11.19	136.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	261	GLU	C-N-CA	11.19	136.40	120.28
1	A	488	VAL	CA-C-N	11.19	136.34	120.79
1	A	488	VAL	C-N-CA	11.19	136.34	120.79
2	B	89	GLY	CA-C-N	11.18	138.33	122.23
2	B	89	GLY	C-N-CA	11.18	138.33	122.23
1	C	430	VAL	CA-CB-CG1	11.15	129.35	110.40
1	C	327	THR	N-CA-C	11.12	127.50	109.72
1	A	627	ASP	N-CA-CB	11.11	128.91	110.47
2	D	524	PHE	CA-CB-CG	11.10	124.90	113.80
2	B	613	ILE	CA-C-O	11.10	132.68	120.59
1	A	265	ASP	CA-CB-CG	11.09	123.69	112.60
2	D	104	MET	CA-C-O	-11.05	108.09	121.02
2	D	24	ALA	CA-C-N	11.04	134.04	120.13
2	D	24	ALA	C-N-CA	11.04	134.04	120.13
2	D	418	LYS	CA-C-O	-11.03	108.72	120.63
1	C	287	PHE	CA-CB-CG	10.99	124.79	113.80
2	B	86	GLY	O-C-N	-10.94	111.12	122.60
2	B	422	GLU	O-C-N	-10.93	108.05	122.59
1	C	412	LEU	O-C-N	-10.87	110.60	122.12
1	A	333	GLY	CA-C-O	10.85	131.93	120.75
1	C	690	GLU	CA-C-N	10.85	135.90	120.28
1	C	690	GLU	C-N-CA	10.85	135.90	120.28
1	C	678	PRO	CA-C-N	10.83	141.44	121.52
1	C	678	PRO	C-N-CA	10.83	141.44	121.52
1	A	327	THR	N-CA-C	10.82	126.95	109.85
1	C	621	TYR	CA-C-N	10.80	135.32	120.63
1	C	621	TYR	C-N-CA	10.80	135.32	120.63
2	D	238	ALA	O-C-N	-10.79	109.59	122.22
2	D	338	VAL	CA-C-N	10.78	135.80	120.28
2	D	338	VAL	C-N-CA	10.78	135.80	120.28
2	B	148	GLU	CA-C-O	-10.77	109.14	120.55
1	A	521	ASN	OD1-CG-ND2	10.73	133.34	122.60
1	A	241	SER	N-CA-C	10.72	127.37	110.32
1	A	651	VAL	N-CA-C	10.72	122.50	108.35
1	A	665	VAL	CA-C-O	10.71	125.86	118.69
2	B	483	PRO	CA-C-O	-10.70	109.14	121.34
2	B	20	THR	CA-C-O	-10.70	102.61	120.80
2	B	274	THR	O-C-N	-10.70	110.78	122.12
2	B	435	THR	CA-CB-CG2	10.69	128.67	110.50
2	B	327	SER	CA-C-O	10.67	132.97	120.70
1	A	592	GLN	CB-CG-CD	10.64	130.70	112.60
2	D	95	ARG	CG-CD-NE	10.59	135.29	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	370	PRO	CA-C-O	10.57	133.39	121.34
1	A	574	VAL	CB-CA-C	10.56	124.09	111.32
2	D	311	PHE	CA-C-N	10.55	136.05	120.11
2	D	311	PHE	C-N-CA	10.55	136.05	120.11
1	A	287	PHE	CA-CB-CG	10.55	124.35	113.80
2	D	405	VAL	CA-C-O	-10.54	110.00	121.17
2	B	77	ARG	CA-C-O	10.53	131.51	120.66
1	A	123	ARG	CD-NE-CZ	10.53	139.14	124.40
2	D	47	ARG	CD-NE-CZ	10.53	139.14	124.40
1	C	241	SER	N-CA-C	10.52	126.56	109.72
1	C	262	ASP	O-C-N	-10.52	111.15	122.09
1	A	720	LYS	CA-C-N	10.52	134.12	120.44
1	A	720	LYS	C-N-CA	10.52	134.12	120.44
1	C	115	VAL	N-CA-C	10.52	122.78	108.89
1	C	456	ARG	NE-CZ-NH1	10.52	132.01	121.50
2	D	86	GLY	O-C-N	-10.51	109.03	122.70
1	C	528	ASP	CA-C-N	10.51	139.88	122.54
1	C	528	ASP	C-N-CA	10.51	139.88	122.54
2	B	521	ARG	O-C-N	-10.48	111.01	122.12
1	A	268	ARG	NE-CZ-NH2	-10.48	109.77	119.20
2	D	89	GLY	CA-C-N	10.46	140.81	121.97
2	D	89	GLY	C-N-CA	10.46	140.81	121.97
1	C	262	ASP	CA-C-N	10.46	131.81	119.99
1	C	262	ASP	C-N-CA	10.46	131.81	119.99
1	C	261	ALA	O-C-N	-10.46	111.30	122.07
2	D	544	GLN	CA-CB-CG	10.45	135.00	114.10
2	B	238	ALA	CA-C-N	10.44	135.32	120.28
2	B	238	ALA	C-N-CA	10.44	135.32	120.28
1	A	313	HIS	O-C-N	-10.43	108.83	122.39
1	C	697	ARG	CA-C-N	10.39	134.62	120.38
1	C	697	ARG	C-N-CA	10.39	134.62	120.38
2	B	466	PHE	O-C-N	-10.38	116.76	121.53
1	A	244	ALA	CA-C-N	10.37	133.92	120.44
1	A	244	ALA	C-N-CA	10.37	133.92	120.44
2	B	146	ALA	CA-C-N	10.36	130.55	119.05
2	B	146	ALA	C-N-CA	10.36	130.55	119.05
1	A	633	LEU	O-C-N	-10.35	110.47	122.68
2	D	293	THR	O-C-N	-10.35	111.16	122.12
1	C	633	LEU	O-C-N	-10.34	109.93	122.65
2	D	574	TYR	CA-C-N	10.33	133.86	120.44
2	D	574	TYR	C-N-CA	10.33	133.86	120.44
1	A	319	ASN	CA-CB-CG	10.31	122.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	237	ASP	CA-CB-CG	10.29	122.89	112.60
1	C	246	GLN	O-C-N	-10.27	111.49	122.07
2	D	86	GLY	CA-C-O	10.27	138.44	120.57
2	D	48	PRO	O-C-N	-10.25	116.59	121.31
1	A	126	ASP	CA-CB-CG	10.24	122.84	112.60
2	B	362	PRO	N-CA-CB	10.24	113.02	103.39
1	C	80	ALA	O-C-N	-10.24	111.26	122.12
1	C	54	VAL	CA-C-O	-10.23	110.41	121.05
1	C	401	ASP	CA-C-O	10.22	134.16	120.16
2	B	191	LYS	CA-C-N	10.21	138.85	122.11
2	B	191	LYS	C-N-CA	10.21	138.85	122.11
2	B	623	VAL	CA-C-N	10.20	133.41	120.56
2	B	623	VAL	C-N-CA	10.20	133.41	120.56
2	B	232	ARG	CD-NE-CZ	10.20	138.68	124.40
1	A	231	ASN	O-C-N	-10.20	110.17	122.20
1	A	727	ASP	CA-C-N	10.17	140.01	121.70
1	A	727	ASP	C-N-CA	10.17	140.01	121.70
1	C	553	GLU	CA-C-N	10.17	134.92	120.79
1	C	553	GLU	C-N-CA	10.17	134.92	120.79
2	B	307	ILE	CA-C-N	10.16	132.93	120.13
2	B	307	ILE	C-N-CA	10.16	132.93	120.13
1	A	304	ALA	O-C-N	-10.16	111.35	122.12
2	B	490	TRP	O-C-N	-10.12	111.33	123.27
1	C	683	THR	N-CA-CB	10.12	128.39	111.08
1	A	89	TYR	CA-C-O	-10.12	109.83	121.16
1	A	662	LEU	CA-C-O	-10.11	108.67	120.10
1	C	456	ARG	CD-NE-CZ	10.07	138.50	124.40
1	A	402	PRO	O-C-N	-10.04	110.69	122.24
1	C	704	ILE	O-C-N	-10.04	112.74	123.18
1	C	541	ALA	CA-C-N	10.04	140.72	121.54
1	C	541	ALA	C-N-CA	10.04	140.72	121.54
1	A	520	GLY	O-C-N	-10.02	111.35	122.28
1	A	485	ASN	CB-CA-C	-10.02	94.16	110.79
1	A	372	ILE	CA-C-O	-10.01	111.89	120.80
1	C	333	GLY	CA-C-N	10.01	134.05	120.54
1	C	333	GLY	C-N-CA	10.01	134.05	120.54
1	C	182	ALA	CA-C-N	10.00	137.09	121.19
1	C	182	ALA	C-N-CA	10.00	137.09	121.19
2	B	492	ARG	CD-NE-CZ	9.99	138.38	124.40
1	A	690	GLU	O-C-N	-9.98	110.82	122.20
1	C	184	GLU	CA-C-N	9.98	140.62	122.06
1	C	184	GLU	C-N-CA	9.98	140.62	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	PRO	O-C-N	-9.96	109.19	122.64
1	C	627	ASP	N-CA-CB	9.95	126.65	110.43
2	D	515	LEU	CA-C-O	9.94	130.99	120.36
2	B	397	ASP	CA-C-O	9.92	128.20	120.26
2	B	337	TYR	CA-C-N	9.89	136.09	120.47
2	B	337	TYR	C-N-CA	9.89	136.09	120.47
1	C	367	SER	CA-C-O	9.88	132.94	121.28
2	D	380	ARG	CD-NE-CZ	9.88	138.23	124.40
2	B	524	PHE	CA-CB-CG	9.87	123.67	113.80
1	A	333	GLY	CA-C-N	9.87	133.90	120.38
1	A	333	GLY	C-N-CA	9.87	133.90	120.38
2	D	44	ASN	CA-CB-CG	-9.83	102.77	112.60
2	D	622	ASP	CA-CB-CG	9.83	122.43	112.60
1	C	70	PHE	CA-CB-CG	9.82	123.62	113.80
1	C	518	ALA	CA-C-O	-9.82	110.14	120.55
2	D	425	LYS	CA-C-N	9.80	138.72	122.54
2	D	425	LYS	C-N-CA	9.80	138.72	122.54
1	C	550	ASP	N-CA-C	-9.79	100.56	111.14
2	D	425	LYS	O-C-N	-9.77	109.68	122.39
2	D	25	GLY	O-C-N	-9.77	112.13	122.19
2	D	531	SER	CA-C-O	9.76	131.25	121.00
2	B	602	PHE	CA-C-N	9.75	140.52	121.41
2	B	602	PHE	C-N-CA	9.75	140.52	121.41
1	A	667	ALA	CA-C-N	9.75	133.69	120.44
1	A	667	ALA	C-N-CA	9.75	133.69	120.44
2	B	25	GLY	O-C-N	-9.74	110.03	122.70
1	A	647	ALA	CA-C-O	9.74	130.25	119.15
1	C	272	SER	CA-C-O	-9.71	109.32	120.20
2	D	632	ASP	O-C-N	-9.69	111.71	122.08
1	C	394	SER	CA-C-O	9.68	131.04	120.10
1	C	485	ASN	CB-CA-C	-9.68	95.68	110.88
1	C	205	MET	CA-C-O	-9.68	110.16	120.42
1	C	394	SER	N-CA-C	9.68	122.84	111.71
1	A	343	ASN	CA-C-N	9.67	134.21	120.28
1	A	343	ASN	C-N-CA	9.67	134.21	120.28
2	B	422	GLU	CA-C-N	9.67	134.15	120.42
2	B	422	GLU	C-N-CA	9.67	134.15	120.42
1	C	594	GLU	CB-CG-CD	9.66	129.03	112.60
1	C	674	LYS	O-C-N	-9.66	109.77	122.33
1	A	180	VAL	CA-C-N	9.65	133.60	120.38
1	A	180	VAL	C-N-CA	9.65	133.60	120.38
2	B	601	GLU	CA-C-N	9.64	144.09	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GLU	C-N-CA	9.64	144.09	121.52
2	D	190	ALA	CA-C-O	-9.64	110.58	120.90
1	A	475	GLU	CA-C-O	9.64	127.57	119.66
2	B	251	GLU	CB-CG-CD	9.63	128.98	112.60
2	D	329	ARG	CA-C-N	9.62	136.78	120.72
2	D	329	ARG	C-N-CA	9.62	136.78	120.72
1	C	129	ASN	CA-C-O	9.59	128.98	119.49
1	C	674	LYS	CA-C-N	9.59	139.74	122.38
1	C	674	LYS	C-N-CA	9.59	139.74	122.38
2	B	416	ALA	CA-C-N	9.59	133.31	120.65
2	B	416	ALA	C-N-CA	9.59	133.31	120.65
1	C	369	ASP	O-C-N	-9.58	110.03	122.39
2	D	243	ASN	O-C-N	-9.58	109.85	122.59
1	A	319	ASN	CA-C-O	9.57	130.04	119.32
2	D	435	THR	CA-CB-CG2	9.56	126.75	110.50
1	A	219	ARG	NH1-CZ-NH2	9.55	131.72	119.30
1	C	312	VAL	O-C-N	-9.54	112.23	121.87
1	C	665	VAL	CA-C-N	9.54	129.78	119.28
1	C	665	VAL	C-N-CA	9.54	129.78	119.28
1	C	427	VAL	CA-C-O	-9.53	108.87	120.78
2	B	600	LYS	CA-C-N	9.52	133.43	120.38
2	B	600	LYS	C-N-CA	9.52	133.43	120.38
2	B	444	ALA	CA-C-N	9.52	132.81	120.44
2	B	444	ALA	C-N-CA	9.52	132.81	120.44
1	A	149	MET	CA-C-N	9.49	133.00	120.28
1	A	149	MET	C-N-CA	9.49	133.00	120.28
2	D	190	ALA	O-C-N	-9.49	112.22	122.09
1	A	354	ALA	O-C-N	9.49	131.84	122.07
1	A	640	THR	CA-C-N	9.47	133.15	120.65
1	A	640	THR	C-N-CA	9.47	133.15	120.65
2	D	315	GLU	O-C-N	-9.44	110.03	122.59
2	D	67	VAL	O-C-N	-9.44	112.50	121.94
2	B	460	ILE	N-CA-CB	9.43	124.17	112.10
1	C	159	ASP	CA-CB-CG	9.43	122.03	112.60
1	C	216	PRO	CA-C-N	9.43	132.70	120.44
1	C	216	PRO	C-N-CA	9.43	132.70	120.44
2	B	515	LEU	CA-C-N	9.43	137.34	122.26
2	B	515	LEU	C-N-CA	9.43	137.34	122.26
2	D	205	ALA	N-CA-C	-9.42	100.70	110.97
2	D	410	ARG	O-C-N	-9.40	112.39	122.07
1	A	619	THR	CA-C-N	9.39	133.22	120.44
1	A	619	THR	C-N-CA	9.39	133.22	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	GLU	CB-CG-CD	9.38	128.54	112.60
2	D	635	GLY	CA-C-N	-9.37	109.51	122.91
2	D	635	GLY	C-N-CA	-9.37	109.51	122.91
2	B	378	ILE	O-C-N	-9.37	112.73	121.91
1	A	405	GLY	O-C-N	-9.36	110.54	122.70
2	B	403	TYR	O-C-N	-9.35	112.44	122.07
1	A	714	SER	CA-C-N	9.33	133.13	120.44
1	A	714	SER	C-N-CA	9.33	133.13	120.44
2	B	117	ASP	CA-CB-CG	9.32	121.92	112.60
2	D	457	LYS	CA-C-O	9.32	130.56	119.28
1	A	416	LEU	O-C-N	-9.31	112.25	122.12
1	A	54	VAL	CA-C-O	-9.31	108.77	120.03
1	C	448	GLU	CA-C-N	9.31	133.11	120.54
1	C	448	GLU	C-N-CA	9.31	133.11	120.54
1	A	652	VAL	N-CA-CB	9.31	122.77	111.60
1	C	43	GLN	CA-C-O	9.30	132.53	121.65
1	A	554	LYS	CB-CG-CD	9.30	132.68	111.30
1	C	667	ALA	O-C-N	-9.29	111.55	122.15
2	B	633	ILE	O-C-N	-9.29	110.96	122.57
2	B	78	PRO	O-C-N	-9.29	112.15	122.18
2	D	48	PRO	CA-C-N	9.29	130.24	119.47
2	D	48	PRO	C-N-CA	9.29	130.24	119.47
1	C	231	ASN	O-C-N	-9.28	112.13	122.34
1	C	343	ASN	O-C-N	-9.28	111.36	122.22
2	B	160	GLU	CB-CG-CD	9.28	128.37	112.60
1	A	661	HIS	O-C-N	-9.27	111.45	122.11
1	A	592	GLN	CB-CA-C	-9.27	95.40	110.79
2	D	483	PRO	CA-C-O	-9.27	110.77	121.34
1	C	523	ASP	N-CA-CB	9.27	125.36	110.90
1	C	369	ASP	CA-C-N	9.26	133.90	120.38
1	C	369	ASP	C-N-CA	9.26	133.90	120.38
1	C	104	ARG	CD-NE-CZ	9.26	137.36	124.40
2	D	172	GLN	N-CA-C	9.26	121.37	111.28
1	A	603	ALA	N-CA-C	9.24	124.46	109.59
1	A	23	ARG	CD-NE-CZ	9.23	137.33	124.40
1	C	277	VAL	O-C-N	-9.23	112.84	121.89
2	D	146	ALA	CA-C-N	9.23	129.84	119.32
2	D	146	ALA	C-N-CA	9.23	129.84	119.32
2	B	47	ARG	NE-CZ-NH1	9.22	130.72	121.50
2	D	188	LYS	N-CA-C	-9.21	96.00	110.10
2	D	363	PHE	CA-CB-CG	9.21	123.00	113.80
1	A	258	TYR	CA-C-O	-9.20	110.80	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	292	LEU	N-CA-C	-9.20	101.20	111.14
2	D	457	LYS	O-C-N	-9.20	109.67	122.37
1	C	703	GLU	CA-C-N	9.20	136.04	122.98
1	C	703	GLU	C-N-CA	9.20	136.04	122.98
1	C	464	LEU	CA-C-O	9.19	129.38	120.09
1	A	665	VAL	CA-C-N	9.16	129.22	119.05
1	A	665	VAL	C-N-CA	9.16	129.22	119.05
1	C	231	ASN	CA-C-O	9.15	128.92	118.77
1	A	216	PRO	CA-C-N	9.14	132.53	120.28
1	A	216	PRO	C-N-CA	9.14	132.53	120.28
2	B	276	ALA	N-CA-C	-9.14	100.88	111.03
1	C	19	ALA	CA-C-N	9.14	136.86	122.60
1	C	19	ALA	C-N-CA	9.14	136.86	122.60
1	C	120	PRO	O-C-N	-9.13	112.31	122.18
1	C	267	ILE	N-CA-C	-9.12	101.85	110.42
1	A	343	ASN	O-C-N	-9.10	111.57	122.22
2	B	75	MET	O-C-N	-9.10	112.66	123.31
2	B	162	THR	N-CA-C	9.10	123.73	108.90
2	B	314	ASP	CA-CB-CG	9.08	121.68	112.60
2	B	516	ALA	CA-C-N	-9.08	108.44	121.42
2	B	516	ALA	C-N-CA	-9.08	108.44	121.42
2	D	61	ARG	CD-NE-CZ	9.07	137.10	124.40
1	A	222	SER	O-C-N	-9.07	112.51	122.12
2	B	338	VAL	O-C-N	-9.06	112.72	121.87
2	D	422	GLU	CA-C-N	9.06	133.29	120.42
2	D	422	GLU	C-N-CA	9.06	133.29	120.42
2	D	223	ARG	NE-CZ-NH1	9.05	130.55	121.50
1	A	612	ARG	CA-C-N	9.04	129.80	119.94
1	A	612	ARG	C-N-CA	9.04	129.80	119.94
1	C	35	GLY	CA-C-O	-9.04	112.24	121.64
1	C	711	ILE	CA-C-N	9.04	128.37	118.97
1	C	711	ILE	C-N-CA	9.04	128.37	118.97
2	D	147	PRO	CA-C-N	9.03	136.94	121.14
2	D	147	PRO	C-N-CA	9.03	136.94	121.14
2	D	408	LEU	CA-C-N	9.03	132.72	120.44
2	D	408	LEU	C-N-CA	9.03	132.72	120.44
2	D	288	HIS	CA-CB-CG	9.02	122.82	113.80
1	A	537	ASP	CA-CB-CG	9.01	121.61	112.60
1	A	573	GLU	CA-C-O	-9.01	107.63	120.51
2	D	337	TYR	O-C-N	-9.00	111.69	122.22
1	C	521	ASN	N-CA-C	9.00	125.34	108.97
2	B	339	ASN	CA-C-N	8.99	133.19	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	339	ASN	C-N-CA	8.99	133.19	120.42
1	A	277	VAL	O-C-N	-8.99	111.34	122.57
2	D	228	SER	CA-C-N	8.99	128.64	119.56
2	D	228	SER	C-N-CA	8.99	128.64	119.56
1	C	146	ILE	O-C-N	-8.97	112.81	121.87
2	B	146	ALA	CA-C-O	8.97	128.67	120.60
2	D	365	GLN	N-CA-C	8.96	123.98	112.34
2	D	288	HIS	CB-CG-CD2	8.96	142.84	131.20
1	A	339	GLN	OE1-CD-NE2	-8.95	113.65	122.60
2	B	268	GLU	O-C-N	-8.94	112.51	122.08
2	D	256	LEU	CA-C-N	8.94	132.61	120.54
2	D	256	LEU	C-N-CA	8.94	132.61	120.54
2	B	55	PHE	CA-C-N	8.94	132.63	120.38
2	B	55	PHE	C-N-CA	8.94	132.63	120.38
2	B	305	ALA	CA-C-N	8.93	132.98	120.29
2	B	305	ALA	C-N-CA	8.93	132.98	120.29
1	C	699	ASP	CA-CB-CG	8.91	121.52	112.60
1	A	261	ALA	O-C-N	-8.91	111.31	122.27
1	A	627	ASP	CA-C-O	8.90	129.98	120.46
2	D	203	GLY	CA-C-N	8.88	132.18	120.28
2	D	203	GLY	C-N-CA	8.88	132.18	120.28
2	D	248	ASP	CA-CB-CG	-8.88	103.72	112.60
2	B	227	PHE	N-CA-CB	-8.87	97.76	110.44
1	A	638	GLU	O-C-N	-8.86	112.94	122.07
2	D	394	ARG	CD-NE-CZ	8.86	136.81	124.40
1	C	314	GLN	O-C-N	-8.86	110.81	122.59
2	B	59	LEU	O-C-N	-8.86	112.82	122.03
1	C	623	ASP	O-C-N	-8.86	110.81	122.33
2	D	629	SER	O-C-N	-8.85	112.89	122.09
2	B	154	LEU	CA-C-N	8.83	134.06	120.82
2	B	154	LEU	C-N-CA	8.83	134.06	120.82
1	C	589	GLU	O-C-N	-8.82	111.96	122.11
2	B	498	GLU	CB-CG-CD	8.82	127.59	112.60
2	D	24	ALA	CA-C-O	8.82	129.77	120.42
2	B	66	THR	O-C-N	-8.82	111.89	122.65
2	D	391	ASN	CA-CB-CG	-8.81	103.79	112.60
1	A	394	SER	N-CA-C	8.80	122.03	111.82
2	B	496	VAL	O-C-N	-8.80	113.14	121.94
2	B	599	PHE	O-C-N	-8.80	111.93	122.22
2	B	407	SER	O-C-N	-8.79	113.01	122.07
1	A	226	ALA	CA-C-O	-8.79	111.49	120.90
1	A	430	VAL	N-CA-CB	-8.79	100.71	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	267	VAL	CA-C-N	8.78	131.86	120.44
2	D	267	VAL	C-N-CA	8.78	131.86	120.44
1	A	281	ALA	O-C-N	-8.78	112.66	120.48
2	B	108	ASP	N-CA-CB	-8.78	96.11	110.42
2	B	128	GLY	CA-C-O	-8.78	111.36	120.66
1	A	371	ALA	CA-C-N	8.77	132.46	123.16
1	A	371	ALA	C-N-CA	8.77	132.46	123.16
1	C	198	ASN	CA-CB-CG	8.77	121.36	112.60
2	D	133	VAL	N-CA-CB	8.76	120.55	110.82
1	A	679	ASP	CA-C-O	-8.76	110.52	120.24
2	D	211	GLU	CA-C-O	8.76	128.48	120.60
2	B	315	GLU	CA-C-N	8.76	137.41	122.26
2	B	315	GLU	C-N-CA	8.76	137.41	122.26
1	C	131	ARG	CA-C-N	8.75	134.71	122.28
1	C	131	ARG	C-N-CA	8.75	134.71	122.28
1	C	320	PRO	N-CA-CB	8.75	111.59	103.46
1	A	357	GLN	CA-C-N	8.74	138.55	121.41
1	A	357	GLN	C-N-CA	8.74	138.55	121.41
1	A	476	PRO	CA-C-N	8.74	128.81	119.90
1	A	476	PRO	C-N-CA	8.74	128.81	119.90
2	B	89	GLY	O-C-N	-8.73	110.73	122.35
1	A	321	LYS	CA-C-N	8.73	132.85	120.28
1	A	321	LYS	C-N-CA	8.73	132.85	120.28
2	D	93	PHE	CA-C-N	8.73	135.07	121.19
2	D	93	PHE	C-N-CA	8.73	135.07	121.19
2	B	160	GLU	CA-C-N	8.73	139.28	122.53
2	B	160	GLU	C-N-CA	8.73	139.28	122.53
1	A	179	VAL	O-C-N	-8.72	113.22	121.94
1	C	385	ASN	O-C-N	-8.71	112.89	122.12
2	D	536	HIS	CA-C-N	8.71	131.84	120.60
2	D	536	HIS	C-N-CA	8.71	131.84	120.60
1	C	726	LEU	N-CA-C	8.71	121.72	111.71
1	C	127	SER	CA-C-O	-8.71	110.26	120.10
2	D	631	LEU	CB-CA-C	8.71	124.66	110.90
1	C	321	LYS	O-C-N	-8.70	111.56	122.27
1	C	643	GLN	OE1-CD-NE2	-8.71	113.89	122.60
1	A	683	THR	N-CA-CB	8.70	124.76	110.85
1	A	207	ARG	CA-C-N	8.69	135.01	122.40
1	A	207	ARG	C-N-CA	8.69	135.01	122.40
2	B	576	GLN	CA-C-O	-8.69	111.95	120.90
2	B	218	GLY	CA-C-N	8.69	138.13	121.54
2	B	218	GLY	C-N-CA	8.69	138.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	191	LYS	CA-C-N	8.69	137.64	122.09
2	D	191	LYS	C-N-CA	8.69	137.64	122.09
1	C	537	ASP	CA-CB-CG	8.68	121.28	112.60
2	B	566	ASP	CA-CB-CG	8.68	121.28	112.60
1	C	603	ALA	N-CA-C	8.68	123.21	109.50
1	C	350	ILE	O-C-N	-8.68	113.41	121.91
1	A	550	ASP	O-C-N	-8.67	113.14	122.07
1	A	533	LYS	CA-C-O	-8.66	111.90	121.00
2	D	185	ARG	CA-C-N	8.66	134.90	122.09
2	D	185	ARG	C-N-CA	8.66	134.90	122.09
2	D	338	VAL	O-C-N	-8.66	113.13	121.87
2	B	50	GLU	CB-CG-CD	8.65	127.31	112.60
1	A	118	ASP	CA-CB-CG	8.65	121.25	112.60
1	C	385	ASN	CA-C-N	8.65	132.21	120.54
1	C	385	ASN	C-N-CA	8.65	132.21	120.54
1	C	623	ASP	CA-CB-CG	8.65	121.25	112.60
2	B	197	LEU	N-CA-C	8.64	120.78	111.36
2	D	606	ALA	N-CA-C	8.64	121.56	111.02
1	C	14	ASN	N-CA-C	8.63	123.99	112.25
1	A	300	LYS	CA-C-N	8.63	131.84	120.28
1	A	300	LYS	C-N-CA	8.63	131.84	120.28
2	D	301	ARG	CA-C-O	-8.62	111.67	120.90
1	A	425	GLN	CA-C-N	8.62	132.18	120.54
1	A	425	GLN	C-N-CA	8.62	132.18	120.54
1	C	575	LYS	CA-C-N	8.62	134.34	122.19
1	C	575	LYS	C-N-CA	8.62	134.34	122.19
1	A	312	VAL	O-C-N	-8.62	112.06	121.80
1	C	662	LEU	CA-C-O	-8.61	110.07	119.97
1	C	211	ILE	CA-C-N	8.61	139.04	121.48
1	C	211	ILE	C-N-CA	8.61	139.04	121.48
1	C	333	GLY	O-C-N	-8.60	113.85	122.19
1	C	123	ARG	CA-C-N	8.59	138.25	121.41
1	C	123	ARG	C-N-CA	8.59	138.25	121.41
1	C	556	PHE	CA-CB-CG	8.59	122.39	113.80
2	D	214	LEU	N-CA-C	8.59	123.32	113.02
1	A	198	ASN	N-CA-CB	-8.58	98.66	111.71
1	C	622	ALA	O-C-N	-8.58	112.77	122.03
1	A	106	LEU	O-C-N	-8.58	113.23	122.07
1	A	411	GLU	CA-C-N	8.57	131.59	120.44
1	A	411	GLU	C-N-CA	8.57	131.59	120.44
2	B	172	GLN	CA-C-N	8.57	129.45	119.94
2	B	172	GLN	C-N-CA	8.57	129.45	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	238	ALA	O-C-N	-8.57	109.92	122.43
2	B	235	THR	N-CA-CB	8.55	124.81	110.87
1	A	139	ALA	CA-C-N	8.55	133.88	120.97
1	A	139	ALA	C-N-CA	8.55	133.88	120.97
2	D	534	VAL	CA-C-N	8.55	131.55	120.44
2	D	534	VAL	C-N-CA	8.55	131.55	120.44
2	D	268	GLU	N-CA-C	-8.54	101.93	111.07
1	A	677	ARG	CA-C-N	8.54	129.27	120.04
1	A	677	ARG	C-N-CA	8.54	129.27	120.04
2	D	48	PRO	CA-C-O	8.54	127.05	120.90
1	A	333	GLY	O-C-N	-8.54	114.00	122.19
1	A	488	VAL	N-CA-CB	8.53	121.48	110.57
1	A	689	PRO	O-C-N	-8.52	112.72	123.03
1	A	646	GLU	CA-C-N	8.52	137.00	122.26
1	A	646	GLU	C-N-CA	8.52	137.00	122.26
2	B	634	LEU	CA-C-N	8.52	138.11	121.41
2	B	634	LEU	C-N-CA	8.52	138.11	121.41
2	B	69	GLY	N-CA-C	8.52	128.02	114.90
1	A	279	GLN	CA-C-O	-8.51	109.05	119.18
1	C	370	GLU	O-C-N	-8.50	112.51	122.20
1	C	44	ILE	CA-C-O	8.50	131.34	119.95
2	B	77	ARG	O-C-N	-8.49	114.13	121.35
1	A	70	PHE	CA-C-O	8.49	131.39	121.54
1	C	236	ASN	CB-CG-ND2	-8.49	103.66	116.40
2	D	490	TRP	CA-C-O	8.48	129.23	120.24
1	C	416	LEU	O-C-N	-8.48	113.27	122.09
1	C	214	PRO	O-C-N	-8.47	111.21	122.64
1	C	319	ASN	CA-C-N	8.46	128.18	119.64
1	C	319	ASN	C-N-CA	8.46	128.18	119.64
2	D	176	ALA	CA-C-N	8.45	132.53	120.79
2	D	176	ALA	C-N-CA	8.45	132.53	120.79
1	A	218	MET	CA-C-N	8.43	131.58	120.28
1	A	218	MET	C-N-CA	8.43	131.58	120.28
2	B	132	GLY	N-CA-C	8.43	126.53	115.40
2	B	466	PHE	CB-CA-C	-8.43	105.22	111.20
1	A	101	PHE	N-CA-C	-8.43	102.05	111.07
1	A	485	ASN	CA-C-O	-8.42	111.63	120.55
2	D	440	LYS	CA-C-N	8.42	131.33	120.56
2	D	440	LYS	C-N-CA	8.42	131.33	120.56
1	C	272	SER	O-C-N	-8.41	112.61	122.20
2	D	75	MET	CA-C-N	8.41	136.94	122.64
2	D	75	MET	C-N-CA	8.41	136.94	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	276	ALA	N-CA-C	-8.41	101.69	111.03
2	B	337	TYR	CA-C-O	-8.40	110.79	120.20
2	D	242	HIS	CA-C-O	-8.39	112.05	120.70
2	B	337	TYR	O-C-N	-8.39	112.64	122.20
1	A	19	ALA	CA-C-N	8.37	136.21	122.73
1	A	19	ALA	C-N-CA	8.37	136.21	122.73
1	A	593	ALA	O-C-N	-8.37	112.60	122.15
1	C	627	ASP	N-CA-C	-8.37	95.60	109.24
1	A	347	ARG	CD-NE-CZ	8.36	136.10	124.40
1	A	375	PRO	N-CA-CB	8.36	110.34	103.32
2	B	498	GLU	CA-C-N	8.36	131.68	120.65
2	B	498	GLU	C-N-CA	8.36	131.68	120.65
2	B	614	ASP	CA-CB-CG	8.36	120.95	112.60
2	D	633	ILE	O-C-N	-8.35	112.13	122.57
1	A	145	SER	O-C-N	-8.35	113.12	122.72
1	C	43	GLN	CA-C-N	8.35	137.57	122.13
1	C	43	GLN	C-N-CA	8.35	137.57	122.13
1	C	281	ALA	O-C-N	-8.34	112.87	120.71
1	C	59	ASP	N-CA-CB	-8.34	97.58	110.92
1	A	639	GLU	CA-CB-CG	8.33	130.77	114.10
2	B	150	LEU	CA-C-N	8.33	131.45	120.28
2	B	150	LEU	C-N-CA	8.33	131.45	120.28
2	D	599	PHE	CA-C-O	-8.33	112.08	120.82
2	D	233	ALA	CA-C-O	8.32	128.20	119.05
1	A	7	PHE	N-CA-C	8.32	123.25	113.18
2	B	245	GLY	CA-C-O	-8.32	110.63	118.95
2	B	353	GLY	CA-C-N	8.32	137.71	121.41
2	B	353	GLY	C-N-CA	8.32	137.71	121.41
1	C	572	LYS	CB-CA-C	-8.31	98.16	110.96
1	A	344	ASN	CA-C-O	-8.31	110.71	120.10
1	A	201	LEU	O-C-N	-8.31	113.32	122.12
1	A	629	ASP	N-CA-CB	8.30	123.58	110.55
2	D	414	ASP	CA-CB-CG	8.30	120.90	112.60
2	B	21	LEU	O-C-N	-8.29	112.67	122.95
1	C	616	VAL	N-CA-C	-8.29	102.74	110.53
2	D	417	TRP	N-CA-C	-8.28	101.83	111.03
2	D	301	ARG	O-C-N	-8.28	113.48	122.09
1	A	678	PRO	N-CA-CB	8.27	111.06	103.20
1	C	207	ARG	N-CA-C	8.27	122.65	112.23
1	C	594	GLU	N-CA-CB	-8.27	98.21	110.53
2	D	292	LEU	CA-C-O	-8.27	112.18	120.70
2	D	499	GLN	OE1-CD-NE2	-8.26	114.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ILE	N-CA-C	-8.26	98.76	107.60
2	B	451	LYS	CA-C-N	8.25	132.01	120.29
2	B	451	LYS	C-N-CA	8.25	132.01	120.29
1	C	27	GLU	CA-C-N	8.25	131.66	120.44
1	C	27	GLU	C-N-CA	8.25	131.66	120.44
2	D	390	VAL	O-C-N	-8.25	112.45	122.18
1	A	352	ALA	O-C-N	-8.24	113.38	122.12
1	C	612	ARG	CA-C-N	8.23	129.06	120.00
1	C	612	ARG	C-N-CA	8.23	129.06	120.00
1	C	497	VAL	N-CA-C	-8.23	102.32	110.30
1	A	314	GLN	CB-CA-C	8.23	124.83	110.85
1	C	491	GLU	CA-C-N	8.22	131.63	120.44
1	C	491	GLU	C-N-CA	8.22	131.63	120.44
1	C	118	ASP	N-CA-CB	8.20	121.45	110.29
1	C	661	HIS	CA-CB-CG	-8.21	105.59	113.80
1	A	70	PHE	CA-CB-CG	8.20	122.00	113.80
2	D	49	PRO	N-CA-C	8.19	125.69	113.81
1	A	469	LYS	O-C-N	-8.19	111.70	122.59
2	D	162	THR	N-CA-C	8.19	122.77	109.59
1	C	52	GLU	CA-C-N	8.18	131.91	120.29
1	C	52	GLU	C-N-CA	8.18	131.91	120.29
1	A	70	PHE	N-CA-C	8.18	122.67	111.54
2	B	559	LYS	CA-C-N	8.18	131.58	120.38
2	B	559	LYS	C-N-CA	8.18	131.58	120.38
2	D	129	LEU	N-CA-CB	8.17	122.26	110.16
1	A	423	HIS	CA-CB-CG	8.17	121.97	113.80
1	A	619	THR	O-C-N	-8.15	113.67	122.07
1	A	53	ASP	N-CA-CB	8.15	122.22	110.16
1	C	369	ASP	CA-CB-CG	8.14	120.75	112.60
1	A	626	PHE	N-CA-CB	-8.14	98.80	110.44
2	D	307	ILE	O-C-N	-8.14	112.39	122.57
1	C	502	GLU	CA-C-O	-8.13	109.66	119.49
1	A	515	ILE	N-CA-C	-8.12	102.62	110.42
2	B	394	ARG	CA-C-N	8.11	133.77	123.14
2	B	394	ARG	C-N-CA	8.11	133.77	123.14
1	A	53	ASP	N-CA-C	-8.11	102.52	111.36
1	A	443	LYS	O-C-N	-8.11	112.74	122.22
1	C	556	PHE	N-CA-C	8.11	123.52	112.90
1	C	677	ARG	O-C-N	-8.11	114.80	121.12
1	C	265	ASP	CA-C-O	-8.10	111.96	120.55
1	C	572	LYS	N-CA-CB	8.10	121.73	109.91
2	B	115	ASP	CA-C-O	8.09	125.69	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	ARG	NE-CZ-NH2	-8.09	111.92	119.20
1	A	556	PHE	N-CA-C	8.08	123.27	113.41
1	C	190	GLU	O-C-N	-8.08	111.31	122.46
2	D	191	LYS	O-C-N	-8.08	111.68	122.43
2	D	232	ARG	NE-CZ-NH2	8.08	126.47	119.20
2	D	408	LEU	O-C-N	-8.08	112.77	122.22
1	A	29	ALA	CA-C-N	8.08	130.94	120.44
1	A	29	ALA	C-N-CA	8.08	130.94	120.44
1	A	412	LEU	O-C-N	-8.07	113.75	122.07
1	C	347	ARG	O-C-N	-8.07	113.70	122.09
2	D	22	SER	CB-CA-C	-8.07	96.56	109.80
1	C	488	VAL	N-CA-CB	8.07	120.90	110.57
2	B	139	ARG	N-CA-CB	8.07	123.68	110.37
2	B	31	THR	CA-C-N	8.06	131.43	120.54
2	B	31	THR	C-N-CA	8.06	131.43	120.54
1	A	163	VAL	CA-C-O	8.06	128.78	120.39
2	D	79	LYS	O-C-N	-8.06	112.84	122.11
2	B	479	PHE	CA-C-N	8.05	128.12	119.90
2	B	479	PHE	C-N-CA	8.05	128.12	119.90
1	C	615	LYS	CA-C-O	8.05	129.29	119.79
1	A	635	GLN	OE1-CD-NE2	-8.05	114.55	122.60
2	B	147	PRO	N-CA-CB	8.05	112.18	103.33
1	A	637	PRO	CA-C-N	8.05	130.90	120.44
1	A	637	PRO	C-N-CA	8.05	130.90	120.44
2	B	100	ARG	CA-C-O	-8.04	111.89	121.05
1	A	133	ALA	CA-C-N	8.03	135.09	120.79
1	A	133	ALA	C-N-CA	8.03	135.09	120.79
2	D	499	GLN	CA-C-O	-8.03	112.39	120.82
2	D	610	GLU	CA-C-N	8.03	131.38	120.54
2	D	610	GLU	C-N-CA	8.03	131.38	120.54
2	D	202	ILE	CA-C-N	8.02	129.05	119.99
2	D	202	ILE	C-N-CA	8.02	129.05	119.99
1	A	183	GLU	CA-C-N	8.02	133.43	120.60
1	A	183	GLU	C-N-CA	8.02	133.43	120.60
1	C	673	ASP	O-C-N	-8.01	113.38	122.03
1	A	315	PHE	CA-CB-CG	-8.01	105.79	113.80
1	A	438	GLU	O-C-N	-8.01	112.86	122.22
1	C	579	GLU	O-C-N	-8.00	112.86	122.22
2	D	239	ASN	O-C-N	-8.00	113.08	122.20
1	A	214	PRO	O-C-N	-8.00	111.84	122.64
2	B	528	GLU	CA-C-O	8.00	128.90	120.42
1	C	596	ARG	NE-CZ-NH1	8.00	129.50	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	GLY	N-CA-C	7.99	127.21	114.90
2	D	24	ALA	O-C-N	-7.99	113.04	122.15
2	B	77	ARG	CA-C-N	7.99	127.55	119.24
2	B	77	ARG	C-N-CA	7.99	127.55	119.24
2	B	79	LYS	CA-C-N	7.99	135.11	121.14
2	B	79	LYS	C-N-CA	7.99	135.11	121.14
1	C	572	LYS	CA-C-O	-7.99	112.61	121.00
1	A	232	MET	CA-C-O	7.98	130.48	121.22
1	C	598	PRO	CB-CA-C	7.98	121.82	111.21
1	A	573	GLU	CA-C-N	-7.97	112.26	123.10
1	A	573	GLU	C-N-CA	-7.97	112.26	123.10
1	C	24	ARG	NE-CZ-NH2	-7.97	112.02	119.20
2	D	418	LYS	O-C-N	-7.97	113.67	122.12
1	C	667	ALA	CA-C-N	7.97	131.61	120.29
1	C	667	ALA	C-N-CA	7.97	131.61	120.29
2	D	286	ALA	N-CA-C	-7.97	95.43	108.41
1	A	99	ASN	CA-C-N	7.96	131.60	120.29
1	A	99	ASN	C-N-CA	7.96	131.60	120.29
1	A	280	PHE	CB-CA-C	7.96	121.31	109.29
2	B	270	GLY	N-CA-C	7.96	127.34	115.08
1	A	554	LYS	CA-C-O	-7.96	112.39	120.90
1	A	668	LEU	N-CA-C	-7.96	102.55	111.14
1	A	392	GLN	N-CA-C	7.95	121.50	111.24
2	D	435	THR	CA-C-O	7.95	131.88	120.51
1	C	413	THR	CA-C-N	7.94	130.76	120.44
1	C	413	THR	C-N-CA	7.94	130.76	120.44
1	A	376	THR	N-CA-C	-7.94	98.47	110.14
1	A	613	GLY	O-C-N	-7.94	114.57	122.19
1	C	529	ARG	N-CA-CB	-7.93	98.75	110.49
2	B	455	ASN	CA-C-N	7.93	133.90	122.40
2	B	455	ASN	C-N-CA	7.93	133.90	122.40
1	A	520	GLY	CA-C-O	7.93	129.02	120.30
1	A	55	TYR	O-C-N	-7.93	112.52	122.27
1	C	25	PHE	N-CA-CB	7.93	121.48	109.98
2	D	93	PHE	O-C-N	-7.92	113.40	121.88
2	B	504	SER	O-C-N	-7.91	112.96	122.22
1	C	353	MET	O-C-N	-7.91	113.73	122.12
1	C	268	ARG	CA-C-O	-7.91	112.44	120.90
2	B	191	LYS	O-C-N	-7.91	112.07	122.59
2	B	394	ARG	CA-C-O	7.90	129.47	119.12
1	A	418	ARG	CA-C-O	-7.90	112.05	120.42
2	B	254	TRP	CA-C-O	-7.88	111.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	SER	CA-C-N	7.88	127.17	118.97
2	B	532	SER	C-N-CA	7.88	127.17	118.97
2	D	139	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	A	515	ILE	CA-C-O	-7.87	112.83	121.17
2	B	360	THR	CA-C-O	-7.87	111.94	120.36
2	D	425	LYS	CA-CB-CG	7.87	129.83	114.10
2	D	204	PHE	CA-C-O	7.86	128.88	120.55
1	A	111	LYS	CA-C-O	-7.86	110.63	119.67
2	B	309	GLU	N-CA-C	-7.86	101.81	111.40
1	A	394	SER	CA-C-O	7.86	129.01	119.97
2	B	274	THR	CA-C-N	7.86	132.26	120.31
2	B	274	THR	C-N-CA	7.86	132.26	120.31
2	D	267	VAL	CA-C-O	7.85	129.17	120.85
1	A	550	ASP	CA-C-N	7.85	131.84	120.38
1	A	550	ASP	C-N-CA	7.85	131.84	120.38
2	B	95	ARG	CG-CD-NE	7.85	129.26	112.00
1	C	443	LYS	CA-C-O	-7.84	111.24	120.10
2	D	223	ARG	CA-C-N	7.84	136.05	122.56
2	D	223	ARG	C-N-CA	7.84	136.05	122.56
1	A	641	ALA	CA-C-N	7.83	131.12	120.54
1	A	641	ALA	C-N-CA	7.83	131.12	120.54
1	C	379	SER	N-CA-C	7.83	119.82	111.28
2	B	404	TYR	CA-C-O	-7.83	112.60	120.82
1	C	534	LEU	CA-C-O	-7.83	112.17	120.63
2	B	189	PRO	N-CA-CB	7.83	111.47	103.25
1	A	636	THR	CA-C-O	7.83	129.64	120.88
1	C	184	GLU	O-C-N	-7.82	112.16	122.33
1	C	158	LEU	O-C-N	-7.82	112.23	122.39
1	C	341	VAL	N-CA-C	7.82	120.82	111.05
1	C	548	MET	CA-C-N	7.81	131.38	120.29
1	C	548	MET	C-N-CA	7.81	131.38	120.29
1	C	504	ASP	CB-CA-C	-7.81	102.44	110.17
1	A	129	ASN	CA-C-N	7.80	127.86	119.28
1	A	129	ASN	C-N-CA	7.80	127.86	119.28
1	A	651	VAL	N-CA-CB	-7.80	98.56	111.36
1	C	70	PHE	O-C-N	-7.80	112.21	122.59
1	C	126	ASP	CA-C-O	7.80	131.02	121.81
2	B	424	GLU	CA-C-N	7.80	130.73	120.28
2	B	424	GLU	C-N-CA	7.80	130.73	120.28
1	A	377	ASP	CA-CB-CG	7.80	120.40	112.60
1	A	5	PRO	CA-C-N	7.79	133.98	123.00
1	A	5	PRO	C-N-CA	7.79	133.98	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	ALA	CA-C-N	7.79	131.05	120.54
2	B	413	ALA	C-N-CA	7.79	131.05	120.54
1	A	203	GLU	O-C-N	-7.79	114.05	122.07
2	D	184	GLU	CB-CG-CD	7.78	125.82	112.60
1	C	109	GLY	N-CA-C	7.78	126.20	115.00
1	C	153	PHE	CA-CB-CG	-7.78	106.02	113.80
2	B	256	LEU	CA-C-N	7.77	132.48	120.82
2	B	256	LEU	C-N-CA	7.77	132.48	120.82
1	C	504	ASP	CA-C-O	7.77	125.89	119.36
1	A	638	GLU	CA-C-N	7.77	131.47	120.28
1	A	638	GLU	C-N-CA	7.77	131.47	120.28
2	D	342	ARG	NE-CZ-NH2	7.77	126.19	119.20
1	A	413	THR	CA-C-N	7.76	131.32	120.29
1	A	413	THR	C-N-CA	7.76	131.32	120.29
1	C	723	ARG	NE-CZ-NH2	-7.76	112.21	119.20
1	A	711	ILE	CA-C-O	7.76	124.61	118.71
1	A	237	SER	N-CA-C	7.75	120.81	111.82
1	C	304	ALA	O-C-N	-7.75	114.03	122.09
2	D	428	GLY	CA-C-O	7.75	128.65	122.52
1	A	429	LYS	O-C-N	-7.75	111.11	122.43
1	C	224	ILE	N-CA-C	-7.75	102.55	111.00
1	C	76	ALA	N-CA-C	7.75	120.41	111.11
1	C	485	ASN	CA-C-O	-7.74	112.69	120.82
1	A	341	VAL	N-CA-C	7.74	121.85	111.17
1	A	319	ASN	CA-C-N	7.73	127.63	119.05
1	A	319	ASN	C-N-CA	7.73	127.63	119.05
2	B	86	GLY	CA-C-O	7.73	130.62	122.59
1	A	466	GLY	CA-C-O	7.72	127.72	119.07
1	C	209	THR	N-CA-CB	7.72	122.74	111.54
1	A	44	ILE	O-C-N	7.72	128.03	120.92
1	A	176	ALA	O-C-N	-7.72	113.82	122.08
1	C	696	LEU	CA-C-O	-7.72	112.37	120.55
2	D	612	LEU	CA-C-O	7.72	128.84	119.97
1	C	672	LEU	CA-C-N	7.71	131.12	120.63
1	C	672	LEU	C-N-CA	7.71	131.12	120.63
2	D	493	ASP	O-C-N	-7.71	113.95	122.12
2	B	143	ASP	CA-CB-CG	7.71	120.31	112.60
2	D	263	VAL	N-CA-C	-7.71	103.34	110.82
1	C	246	GLN	CA-C-O	-7.70	112.73	120.82
1	A	170	ALA	CA-C-N	7.70	130.85	120.77
1	A	170	ALA	C-N-CA	7.70	130.85	120.77
1	A	232	MET	CA-CB-CG	7.69	129.48	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	240	ILE	N-CA-C	-7.69	103.04	110.42
1	A	696	LEU	O-C-N	-7.68	114.10	122.09
1	C	342	TYR	O-C-N	-7.68	111.86	122.46
1	A	126	ASP	O-C-N	-7.68	114.34	122.94
1	C	426	GLU	N-CA-C	-7.67	101.66	111.02
2	D	162	THR	CA-CB-CG2	7.67	123.54	110.50
1	A	521	ASN	N-CA-C	7.67	122.93	108.97
1	C	623	ASP	CA-C-N	7.67	135.20	122.54
1	C	623	ASP	C-N-CA	7.67	135.20	122.54
2	D	316	ASP	CA-CB-CG	7.67	120.27	112.60
1	C	278	ASP	CA-C-O	-7.67	109.08	119.05
2	B	501	MET	O-C-N	-7.67	113.99	122.12
2	B	517	CYS	CA-C-O	-7.67	112.31	121.05
1	C	7	PHE	N-CA-C	7.67	120.71	111.82
2	B	292	LEU	CA-C-N	7.66	130.40	120.44
2	B	292	LEU	C-N-CA	7.66	130.40	120.44
1	A	115	VAL	N-CA-C	7.66	119.61	108.58
2	B	225	ALA	N-CA-C	7.65	122.29	112.34
2	D	117	ASP	CA-CB-CG	7.65	120.25	112.60
2	B	455	ASN	O-C-N	-7.64	113.17	122.34
1	C	55	TYR	O-C-N	-7.64	114.14	122.09
2	D	390	VAL	CA-C-N	7.64	133.48	122.40
2	D	390	VAL	C-N-CA	7.64	133.48	122.40
1	C	28	LEU	N-CA-C	-7.64	102.89	111.14
2	D	54	THR	N-CA-C	-7.64	99.16	110.46
2	D	335	ASP	CA-C-N	7.64	127.53	119.05
2	D	335	ASP	C-N-CA	7.64	127.53	119.05
2	B	85	LEU	CA-C-O	-7.63	109.99	119.38
1	C	551	ALA	CA-C-O	-7.63	111.65	120.20
1	A	252	ALA	CA-C-N	7.62	130.50	120.28
1	A	252	ALA	C-N-CA	7.62	130.50	120.28
1	A	646	GLU	CA-C-O	-7.62	110.62	119.61
2	B	158	LEU	O-C-N	-7.61	112.47	122.59
2	D	120	PHE	CA-C-O	-7.61	113.01	121.00
2	B	386	LEU	CA-C-O	-7.61	112.49	120.55
2	D	200	ASP	CB-CA-C	7.61	121.44	110.87
1	A	416	LEU	CA-C-N	7.60	130.31	120.44
1	A	416	LEU	C-N-CA	7.60	130.31	120.44
1	A	265	ASP	CA-C-O	-7.59	112.37	120.42
2	B	79	LYS	O-C-N	-7.59	112.46	122.33
1	A	300	LYS	CA-C-O	-7.59	112.72	121.07
1	A	495	LYS	CA-C-N	7.59	130.77	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	LYS	C-N-CA	7.59	130.77	120.44
1	A	711	ILE	N-CA-C	7.59	122.16	112.67
2	D	171	ASP	O-C-N	-7.59	112.50	122.59
2	D	298	ARG	CA-C-N	7.59	130.30	120.44
2	D	298	ARG	C-N-CA	7.59	130.30	120.44
2	D	588	ALA	CA-C-O	-7.59	110.66	119.61
2	B	301	ARG	CA-C-O	-7.58	112.86	120.82
2	B	621	MET	CA-C-N	-7.58	112.06	122.30
2	B	621	MET	C-N-CA	-7.58	112.06	122.30
2	D	437	HIS	N-CA-C	7.58	119.62	111.36
2	B	435	THR	CA-CB-OG1	-7.58	98.23	109.60
1	A	579	GLU	N-CA-CB	7.58	122.03	110.28
2	B	23	LEU	CA-C-O	7.58	127.74	119.40
2	D	200	ASP	CA-C-O	7.57	128.89	121.32
2	D	461	THR	CA-C-O	7.57	128.97	120.80
1	C	321	LYS	CA-C-N	7.56	131.42	120.38
1	C	321	LYS	C-N-CA	7.56	131.42	120.38
2	D	473	SER	O-C-N	-7.56	115.04	123.13
1	A	51	ASN	CA-C-O	7.56	130.26	121.49
1	C	232	MET	CA-C-N	7.56	127.20	119.19
1	C	232	MET	C-N-CA	7.56	127.20	119.19
1	A	340	ASP	CA-C-N	7.55	133.00	120.62
1	A	340	ASP	C-N-CA	7.55	133.00	120.62
1	A	670	LYS	CA-C-O	-7.55	112.55	120.55
1	A	389	PHE	CA-C-O	-7.55	112.83	120.90
1	C	252	ALA	N-CA-C	7.55	120.39	111.71
1	C	180	VAL	CB-CA-C	7.54	121.62	111.97
1	A	231	ASN	N-CA-C	7.54	124.92	113.61
2	B	88	PRO	N-CA-CB	7.53	111.74	103.23
1	A	695	GLU	N-CA-C	-7.53	103.01	111.07
2	D	394	ARG	CA-C-O	7.53	128.16	119.35
1	A	99	ASN	O-C-N	-7.53	114.14	122.12
1	A	529	ARG	N-CA-CB	-7.53	99.57	110.56
2	B	523	ASP	CA-C-O	-7.53	110.90	120.31
1	C	311	LEU	O-C-N	-7.53	114.20	122.03
2	D	339	ASN	CA-C-N	7.52	130.76	120.46
2	D	339	ASN	C-N-CA	7.52	130.76	120.46
1	A	580	VAL	CA-C-N	7.52	130.22	120.44
1	A	580	VAL	C-N-CA	7.52	130.22	120.44
1	A	439	LYS	O-C-N	-7.52	110.38	122.41
1	A	693	PHE	N-CA-C	7.52	119.47	111.28
1	C	695	GLU	N-CA-C	-7.52	103.03	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ALA	CA-C-N	7.52	130.69	120.54
1	A	352	ALA	C-N-CA	7.52	130.69	120.54
2	D	435	THR	O-C-N	-7.51	112.60	122.59
1	A	629	ASP	CA-CB-CG	-7.51	105.09	112.60
2	D	282	PHE	CA-CB-CG	7.51	121.31	113.80
1	A	47	GLY	O-C-N	-7.50	116.86	122.71
2	D	128	GLY	CA-C-O	-7.50	112.71	120.66
1	A	690	GLU	CA-C-N	7.50	133.25	120.72
1	A	690	GLU	C-N-CA	7.50	133.25	120.72
1	C	480	VAL	CB-CA-C	-7.50	98.70	110.69
2	D	573	VAL	CA-C-O	-7.49	112.91	120.85
1	C	280	PHE	CB-CA-C	7.49	118.82	109.16
1	A	386	THR	O-C-N	-7.49	114.31	122.09
2	D	521	ARG	O-C-N	-7.49	113.46	122.22
1	A	723	ARG	O-C-N	-7.48	114.08	122.08
2	B	90	VAL	CA-CB-CG2	7.48	123.12	110.40
1	C	5	PRO	N-CA-C	7.48	123.00	111.11
1	A	52	GLU	O-C-N	-7.48	112.64	122.59
2	B	78	PRO	N-CA-CB	7.48	111.30	103.15
2	B	480	PRO	CA-C-O	-7.48	112.91	121.36
2	B	599	PHE	CA-C-N	7.47	131.04	120.28
2	B	599	PHE	C-N-CA	7.47	131.04	120.28
1	C	256	MET	CB-CA-C	-7.47	99.14	110.88
1	C	636	THR	N-CA-C	-7.47	101.34	110.31
1	C	80	ALA	CA-C-O	-7.47	112.56	120.63
2	D	44	ASN	CA-C-N	7.47	131.73	121.05
2	D	44	ASN	C-N-CA	7.47	131.73	121.05
1	C	236	ASN	OD1-CG-ND2	7.47	130.07	122.60
1	C	401	ASP	CA-C-N	7.47	127.83	119.32
1	C	401	ASP	C-N-CA	7.47	127.83	119.32
1	A	672	LEU	CA-C-N	7.46	130.89	120.29
1	A	672	LEU	C-N-CA	7.46	130.89	120.29
2	B	515	LEU	CA-C-O	7.46	128.53	120.32
1	A	434	ALA	CA-C-N	7.46	130.14	120.44
1	A	434	ALA	C-N-CA	7.46	130.14	120.44
2	B	331	LEU	CA-C-O	7.46	129.46	121.55
1	C	429	LYS	O-C-N	-7.46	113.65	122.15
1	C	3	THR	N-CA-CB	7.46	123.09	110.49
1	C	521	ASN	CA-C-O	7.46	130.64	120.80
2	B	220	TRP	N-CA-CB	-7.45	98.84	109.94
1	C	82	ARG	CD-NE-CZ	7.45	134.83	124.40
1	C	592	GLN	N-CA-CB	7.45	121.19	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	SER	CA-C-O	-7.45	113.00	120.82
2	B	308	GLY	O-C-N	-7.45	114.52	122.19
1	C	520	GLY	CA-C-N	7.45	132.94	123.34
1	C	520	GLY	C-N-CA	7.45	132.94	123.34
1	C	577	THR	N-CA-CB	-7.45	99.99	110.04
2	D	301	ARG	CA-C-N	7.44	130.59	120.54
2	D	301	ARG	C-N-CA	7.44	130.59	120.54
2	D	480	PRO	N-CA-CB	7.44	109.80	103.25
1	A	251	THR	O-C-N	-7.44	114.37	122.85
1	C	308	TRP	CA-C-N	7.44	130.25	120.28
1	C	308	TRP	C-N-CA	7.44	130.25	120.28
2	D	339	ASN	O-C-N	-7.44	113.52	122.22
1	A	698	LYS	CA-C-N	7.44	135.84	122.38
1	A	698	LYS	C-N-CA	7.44	135.84	122.38
2	B	457	LYS	CA-C-N	7.43	133.50	123.46
2	B	457	LYS	C-N-CA	7.43	133.50	123.46
1	C	418	ARG	CA-C-O	-7.43	113.25	120.90
2	D	264	ARG	N-CA-C	-7.43	102.88	110.97
2	D	389	GLU	CA-C-N	-7.43	109.81	121.02
2	D	389	GLU	C-N-CA	-7.43	109.81	121.02
1	A	342	TYR	O-C-N	-7.42	112.49	122.43
2	B	521	ARG	CA-C-N	7.42	131.22	120.38
2	B	521	ARG	C-N-CA	7.42	131.22	120.38
1	A	674	LYS	CA-CB-CG	7.42	128.94	114.10
2	B	342	ARG	NE-CZ-NH1	-7.42	114.08	121.50
2	B	521	ARG	CA-CB-CG	7.42	128.94	114.10
1	A	616	VAL	N-CA-C	-7.42	103.63	110.82
1	C	589	GLU	CA-C-N	7.41	130.54	120.54
1	C	589	GLU	C-N-CA	7.41	130.54	120.54
2	B	182	VAL	CA-C-N	7.41	130.07	120.44
2	B	182	VAL	C-N-CA	7.41	130.07	120.44
2	D	410	ARG	CA-C-O	-7.41	113.04	120.82
2	D	156	ASP	CA-CB-CG	-7.41	105.19	112.60
2	B	50	GLU	CA-CB-CG	7.40	128.91	114.10
2	D	327	SER	N-CA-C	7.40	121.12	110.10
2	B	23	LEU	O-C-N	-7.39	114.54	121.79
2	B	267	VAL	N-CA-C	-7.39	103.58	110.53
1	A	505	PRO	N-CA-CB	7.39	110.87	103.48
1	C	123	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	A	581	GLU	N-CA-C	-7.39	103.16	111.07
2	B	335	ASP	CA-C-O	7.39	126.17	120.48
2	B	440	LYS	CA-C-N	7.39	130.13	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	440	LYS	C-N-CA	7.39	130.13	120.60
1	C	394	SER	O-C-N	-7.39	113.57	122.22
1	A	408	TYR	CA-CB-CG	7.38	127.19	113.90
1	A	456	ARG	CD-NE-CZ	7.38	134.73	124.40
2	B	390	VAL	O-C-N	-7.38	113.47	122.18
1	C	487	THR	CA-C-O	-7.38	111.09	119.79
1	C	279	GLN	CA-C-O	-7.37	110.36	119.28
2	B	370	PRO	N-CA-CB	7.37	109.87	103.31
1	C	408	TYR	CA-C-N	7.37	129.85	120.56
1	C	408	TYR	C-N-CA	7.37	129.85	120.56
2	B	243	ASN	O-C-N	-7.37	112.29	122.46
1	C	151	GLU	CA-C-N	7.37	130.48	120.38
1	C	151	GLU	C-N-CA	7.37	130.48	120.38
1	C	367	SER	O-C-N	-7.37	114.63	123.10
1	A	633	LEU	CA-C-O	7.37	130.35	122.03
1	C	409	VAL	O-C-N	-7.37	114.69	121.91
1	A	421	TRP	CA-C-N	7.36	128.11	119.94
1	A	421	TRP	C-N-CA	7.36	128.11	119.94
2	D	342	ARG	CB-CG-CD	7.36	128.22	111.30
1	A	182	ALA	CA-C-N	7.36	130.47	120.54
1	A	182	ALA	C-N-CA	7.36	130.47	120.54
1	A	459	SER	CA-C-N	7.36	135.36	122.05
1	A	459	SER	C-N-CA	7.36	135.36	122.05
2	B	622	ASP	CA-CB-CG	7.36	119.96	112.60
2	D	458	GLN	N-CA-CB	7.36	119.02	110.71
1	C	449	ALA	CA-C-N	7.35	130.73	120.29
1	C	449	ALA	C-N-CA	7.35	130.73	120.29
2	B	32	GLU	CA-C-N	7.35	130.00	120.44
2	B	32	GLU	C-N-CA	7.35	130.00	120.44
2	D	498	GLU	CA-C-N	7.35	130.00	120.44
2	D	498	GLU	C-N-CA	7.35	130.00	120.44
2	B	319	GLY	O-C-N	7.35	129.31	122.99
1	C	58	MET	O-C-N	-7.34	113.90	122.93
1	A	702	VAL	CB-CA-C	-7.34	101.30	111.65
2	B	390	VAL	CA-C-O	7.34	127.64	119.42
2	D	60	LYS	N-CA-C	-7.34	102.97	110.97
2	B	563	GLN	N-CA-C	-7.34	104.18	113.72
1	A	265	ASP	N-CA-CB	7.34	121.02	110.16
2	B	31	THR	O-C-N	-7.34	113.28	123.11
1	C	671	GLU	CA-C-N	7.34	130.11	120.28
1	C	671	GLU	C-N-CA	7.34	130.11	120.28
2	D	601	GLU	CA-C-N	7.33	135.70	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	GLU	C-N-CA	7.33	135.70	122.06
1	C	395	GLY	CA-C-O	-7.33	109.91	119.44
1	C	522	PRO	CB-CA-C	-7.33	102.59	111.46
2	D	116	PRO	N-CA-CB	7.33	110.95	103.25
1	A	385	ASN	O-C-N	-7.33	114.35	122.12
1	C	647	ALA	CA-C-O	7.33	127.11	119.05
2	D	312	GLY	CA-C-N	7.32	130.53	120.35
2	D	312	GLY	C-N-CA	7.32	130.53	120.35
1	C	591	GLU	CA-C-N	7.32	130.69	120.29
1	C	591	GLU	C-N-CA	7.32	130.69	120.29
1	A	181	THR	CA-C-N	7.32	129.96	120.44
1	A	181	THR	C-N-CA	7.32	129.96	120.44
2	B	394	ARG	NE-CZ-NH2	-7.32	112.61	119.20
2	B	363	PHE	CA-C-N	7.32	135.85	121.58
2	B	363	PHE	C-N-CA	7.32	135.85	121.58
1	A	379	SER	CA-C-O	7.32	128.31	120.55
1	C	171	VAL	CA-C-O	-7.32	113.41	121.17
2	B	85	LEU	CA-C-N	-7.31	112.78	121.85
2	B	85	LEU	C-N-CA	-7.31	112.78	121.85
1	C	453	THR	O-C-N	-7.31	114.26	122.08
2	D	479	PHE	CA-CB-CG	7.31	121.11	113.80
2	D	631	LEU	N-CA-C	-7.31	103.25	111.14
1	A	695	GLU	CA-C-O	-7.30	113.15	120.82
2	D	171	ASP	CA-CB-CG	7.30	119.91	112.60
2	D	524	PHE	N-CA-C	7.30	122.28	113.23
2	D	274	THR	O-C-N	-7.30	112.88	122.59
2	D	374	PHE	CA-C-N	7.30	126.83	119.24
2	D	374	PHE	C-N-CA	7.30	126.83	119.24
2	B	364	THR	CA-C-N	7.30	132.38	120.63
2	B	364	THR	C-N-CA	7.30	132.38	120.63
1	A	91	GLY	O-C-N	-7.30	113.22	122.70
1	A	446	ILE	N-CA-C	-7.30	103.35	110.72
2	B	534	VAL	CA-C-N	7.30	130.06	120.28
2	B	534	VAL	C-N-CA	7.30	130.06	120.28
2	B	107	TRP	N-CA-CB	7.29	121.76	110.46
2	D	33	GLU	CA-C-O	-7.29	113.10	120.90
1	C	401	ASP	O-C-N	-7.29	112.94	121.32
1	C	112	GLY	CA-C-O	-7.29	115.23	121.57
1	C	521	ASN	O-C-N	-7.28	114.79	121.42
1	C	308	TRP	O-C-N	-7.28	114.57	122.07
1	A	562	GLN	O-C-N	-7.27	114.93	123.22
1	A	487	THR	CA-C-O	-7.27	111.61	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	261	GLU	O-C-N	-7.27	113.41	122.20
2	B	423	VAL	CA-C-N	7.27	130.32	120.44
2	B	423	VAL	C-N-CA	7.27	130.32	120.44
1	A	354	ALA	CA-C-O	-7.26	113.20	120.82
1	A	494	ALA	O-C-N	-7.26	112.95	122.39
1	C	79	TYR	CA-C-N	7.26	130.33	120.38
1	C	79	TYR	C-N-CA	7.26	130.33	120.38
1	C	255	GLU	N-CA-C	-7.26	103.30	111.07
1	C	564	ARG	CA-C-O	7.26	129.06	120.20
2	B	560	SER	N-CA-C	7.26	120.11	111.33
2	B	298	ARG	CA-C-N	7.26	130.32	120.38
2	B	298	ARG	C-N-CA	7.26	130.32	120.38
2	D	62	LEU	CA-C-N	7.25	132.42	122.19
2	D	62	LEU	C-N-CA	7.25	132.42	122.19
2	D	137	LEU	CA-C-O	7.25	130.88	120.51
1	C	93	SER	N-CA-CB	-7.25	98.23	110.49
1	A	211	ILE	O-C-N	-7.25	113.51	122.57
1	C	409	VAL	N-CA-C	-7.25	103.47	110.42
2	B	229	PRO	O-C-N	-7.24	112.21	122.35
1	A	262	ASP	CA-C-O	-7.24	113.22	120.82
2	B	340	ILE	CA-C-N	7.23	130.56	120.29
2	B	340	ILE	C-N-CA	7.23	130.56	120.29
2	D	32	GLU	CA-C-N	7.23	130.31	120.54
2	D	32	GLU	C-N-CA	7.23	130.31	120.54
2	B	492	ARG	CG-CD-NE	7.23	127.91	112.00
1	C	131	ARG	O-C-N	-7.23	113.96	122.20
1	C	292	MET	O-C-N	-7.22	112.50	122.46
1	C	433	MET	CA-C-O	-7.22	112.90	120.55
2	D	55	PHE	CA-C-N	7.22	129.82	120.44
2	D	55	PHE	C-N-CA	7.22	129.82	120.44
2	B	458	GLN	N-CA-CB	7.21	123.28	111.30
1	A	545	VAL	N-CA-CB	7.21	118.99	110.55
1	C	312	VAL	CA-C-N	7.21	129.81	120.44
1	C	312	VAL	C-N-CA	7.21	129.81	120.44
1	C	698	LYS	CA-C-O	7.21	128.42	120.63
2	D	208	GLN	CA-C-N	7.21	133.25	121.00
2	D	208	GLN	C-N-CA	7.21	133.25	121.00
2	D	528	GLU	O-C-N	-7.21	114.48	122.12
1	A	176	ALA	CA-C-O	7.21	129.00	121.07
1	A	207	ARG	CG-CD-NE	7.20	127.83	112.00
2	D	398	PRO	O-C-N	-7.20	113.59	122.23
1	A	693	PHE	CA-CB-CG	7.19	120.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	ARG	CA-C-O	-7.19	112.80	120.42
1	C	398	ARG	N-CA-C	7.19	120.03	111.33
2	D	638	LYS	CA-CB-CG	7.19	128.48	114.10
1	A	31	LYS	CA-C-N	7.19	132.90	120.68
1	A	31	LYS	C-N-CA	7.19	132.90	120.68
1	C	8	ASP	O-C-N	-7.19	113.03	122.59
1	C	449	ALA	CA-C-O	7.19	128.59	120.90
1	A	328	HIS	CA-CB-CG	7.19	120.99	113.80
1	C	372	ILE	CA-C-O	-7.19	111.80	120.78
2	B	453	LEU	CA-C-N	7.18	129.91	120.28
2	B	453	LEU	C-N-CA	7.18	129.91	120.28
1	C	594	GLU	CA-CB-CG	7.18	128.47	114.10
2	B	25	GLY	CA-C-N	7.18	133.71	121.14
2	B	25	GLY	C-N-CA	7.18	133.71	121.14
2	B	455	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	C	282	PRO	CA-C-N	7.18	134.14	122.65
1	C	282	PRO	C-N-CA	7.18	134.14	122.65
1	A	379	SER	N-CA-C	7.18	119.11	111.28
1	A	334	TRP	CA-C-N	7.18	132.71	120.72
1	A	334	TRP	C-N-CA	7.18	132.71	120.72
2	D	130	GLU	CA-C-N	7.18	135.25	121.54
2	D	130	GLU	C-N-CA	7.18	135.25	121.54
1	A	145	SER	CA-C-N	7.18	129.86	120.60
1	A	145	SER	C-N-CA	7.18	129.86	120.60
1	C	8	ASP	N-CA-C	7.18	126.09	110.80
1	C	66	GLY	CA-C-N	7.17	135.40	122.13
1	C	66	GLY	C-N-CA	7.17	135.40	122.13
1	C	344	ASN	CA-C-N	7.17	129.60	120.56
1	C	344	ASN	C-N-CA	7.17	129.60	120.56
2	D	229	PRO	O-C-N	-7.17	112.55	122.30
2	D	344	SER	N-CA-C	7.17	119.10	111.28
2	D	407	SER	O-C-N	-7.17	113.52	122.20
2	D	180	VAL	N-CA-CB	7.17	121.33	110.58
1	C	146	ILE	CA-C-N	7.16	130.75	120.79
1	C	146	ILE	C-N-CA	7.16	130.75	120.79
1	C	158	LEU	CA-C-N	7.16	132.85	120.68
1	C	158	LEU	C-N-CA	7.16	132.85	120.68
1	C	677	ARG	CA-CB-CG	7.16	128.42	114.10
2	B	394	ARG	NH1-CZ-NH2	7.16	128.61	119.30
2	D	120	PHE	N-CA-C	-7.16	103.17	110.97
1	A	471	ARG	CA-CB-CG	7.16	128.41	114.10
1	A	123	ARG	CA-C-N	7.15	133.67	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	C-N-CA	7.15	133.67	120.87
1	C	133	ALA	O-C-N	-7.15	113.08	122.59
2	D	602	PHE	CA-C-N	7.15	135.43	121.41
2	D	602	PHE	C-N-CA	7.15	135.43	121.41
1	A	522	PRO	CA-C-N	-7.15	111.75	122.47
1	A	522	PRO	C-N-CA	-7.15	111.75	122.47
2	D	450	ALA	CA-C-N	7.15	130.16	120.44
2	D	450	ALA	C-N-CA	7.15	130.16	120.44
2	B	180	VAL	N-CA-CB	7.15	120.26	110.54
1	C	698	LYS	N-CA-C	7.15	119.98	111.33
2	B	200	ASP	CA-CB-CG	7.14	119.75	112.60
1	C	206	VAL	CA-CB-CG1	7.14	122.55	110.40
2	D	559	LYS	CA-C-N	7.14	130.56	120.28
2	D	559	LYS	C-N-CA	7.14	130.56	120.28
2	B	491	HIS	CA-CB-CG	7.14	120.94	113.80
1	A	215	GLN	O-C-N	-7.13	113.12	121.32
1	C	588	GLU	O-C-N	-7.13	114.72	122.07
1	A	687	VAL	CA-C-N	7.13	129.06	122.85
1	A	687	VAL	C-N-CA	7.13	129.06	122.85
1	A	8	ASP	CA-C-N	7.13	134.26	121.92
1	A	8	ASP	C-N-CA	7.13	134.26	121.92
2	B	578	GLY	CA-C-O	7.13	132.98	120.57
1	C	712	PRO	N-CA-CB	7.13	110.86	103.23
2	D	466	PHE	CB-CA-C	-7.13	106.14	111.20
1	C	237	SER	N-CA-C	7.13	121.56	113.01
2	D	358	ILE	CB-CG1-CD1	7.12	128.76	113.80
1	A	398	ARG	N-CA-C	7.12	119.90	111.71
2	D	82	PRO	N-CA-CB	7.12	109.30	103.32
1	A	198	ASN	OD1-CG-ND2	7.12	129.72	122.60
2	D	223	ARG	CB-CG-CD	7.12	127.66	111.30
2	B	500	LEU	CA-C-O	-7.11	113.35	120.82
1	A	498	LYS	CB-CG-CD	7.11	127.65	111.30
2	B	273	ALA	N-CA-C	-7.11	103.57	111.82
1	A	231	ASN	CA-C-O	7.11	127.56	119.18
1	C	597	ARG	CD-NE-CZ	7.11	134.35	124.40
2	D	229	PRO	N-CA-CB	7.10	110.33	103.51
1	A	666	PRO	O-C-N	-7.10	113.71	122.23
1	C	495	LYS	CA-C-N	7.10	132.72	120.58
1	C	495	LYS	C-N-CA	7.10	132.72	120.58
1	A	267	ILE	CA-C-N	7.09	129.66	120.44
1	A	267	ILE	C-N-CA	7.09	129.66	120.44
1	A	439	LYS	CA-C-N	7.09	136.71	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	LYS	C-N-CA	7.09	136.71	121.18
2	B	327	SER	N-CA-C	7.09	120.52	109.96
1	C	27	GLU	O-C-N	-7.08	113.93	122.22
1	A	175	LEU	CA-C-N	7.08	130.63	120.79
1	A	175	LEU	C-N-CA	7.08	130.63	120.79
1	A	190	GLU	O-C-N	-7.08	112.94	122.43
2	D	493	ASP	N-CA-C	7.08	119.89	111.33
1	A	664	LEU	N-CA-C	7.08	118.64	111.07
2	B	263	VAL	N-CA-C	-7.07	103.89	110.53
1	C	12	LEU	CA-C-O	-7.07	113.40	120.82
1	C	405	GLY	CA-C-O	-7.07	111.92	119.55
2	B	286	ALA	N-CA-CB	7.07	122.20	110.47
1	C	421	TRP	CA-C-O	7.07	128.09	120.10
2	B	117	ASP	CA-C-N	7.06	129.75	120.28
2	B	117	ASP	C-N-CA	7.06	129.75	120.28
2	D	268	GLU	CA-C-O	-7.06	113.40	120.82
1	A	17	VAL	CA-C-O	7.06	124.36	119.20
2	D	490	TRP	N-CA-CB	-7.06	99.69	110.77
1	C	30	ALA	O-C-N	-7.06	114.75	122.09
1	A	8	ASP	N-CA-C	7.06	120.99	112.38
1	A	321	LYS	O-C-N	-7.05	113.22	122.39
2	D	123	LYS	CA-C-N	7.05	130.06	120.54
2	D	123	LYS	C-N-CA	7.05	130.06	120.54
1	C	98	SER	CA-C-N	7.05	129.61	120.44
1	C	98	SER	C-N-CA	7.05	129.61	120.44
1	C	278	ASP	CA-CB-CG	-7.05	105.55	112.60
2	D	91	ALA	CA-C-O	7.05	129.82	120.16
1	C	526	ASP	CA-C-O	7.05	126.75	119.49
1	A	178	TYR	N-CA-C	-7.04	103.53	111.07
2	D	636	VAL	CB-CA-C	7.04	120.91	110.98
1	C	19	ALA	N-CA-C	7.04	120.97	112.38
1	C	513	ASP	CA-C-N	7.04	129.59	120.44
1	C	513	ASP	C-N-CA	7.04	129.59	120.44
1	C	616	VAL	N-CA-CB	7.03	119.57	110.57
2	B	269	GLN	O-C-N	-7.03	113.25	122.59
2	D	351	SER	O-C-N	-7.03	114.78	122.09
2	D	397	ASP	CA-CB-CG	7.03	119.62	112.60
1	C	131	ARG	NE-CZ-NH2	-7.02	112.88	119.20
1	C	421	TRP	O-C-N	-7.02	114.01	122.22
2	D	416	ALA	CA-C-N	7.02	130.18	120.63
2	D	416	ALA	C-N-CA	7.02	130.18	120.63
2	D	560	SER	O-C-N	-7.02	114.01	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	LYS	N-CA-C	-7.01	103.68	111.82
2	D	363	PHE	CA-C-N	7.01	135.26	121.58
2	D	363	PHE	C-N-CA	7.01	135.26	121.58
1	A	264	VAL	O-C-N	-7.01	115.07	121.87
1	C	409	VAL	CA-C-O	-7.01	113.74	121.17
1	C	179	VAL	O-C-N	-7.00	115.05	121.91
2	D	492	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	A	308	TRP	CA-C-N	6.99	129.98	120.54
1	A	308	TRP	C-N-CA	6.99	129.98	120.54
1	A	319	ASN	CB-CG-ND2	6.99	126.88	116.40
1	A	674	LYS	CA-C-O	-6.99	111.93	119.97
2	B	500	LEU	O-C-N	-6.99	114.87	122.07
2	D	404	TYR	CA-C-O	-6.99	113.42	120.90
2	B	612	LEU	CA-C-O	6.99	127.49	119.18
1	C	352	ALA	O-C-N	-6.98	114.88	122.07
2	B	438	VAL	CA-C-N	6.97	129.50	120.44
2	B	438	VAL	C-N-CA	6.97	129.50	120.44
2	B	107	TRP	N-CA-C	-6.97	100.15	110.46
1	C	150	ARG	CA-C-N	6.97	129.50	120.44
1	C	150	ARG	C-N-CA	6.97	129.50	120.44
1	C	454	GLN	CA-C-N	6.96	129.50	120.44
1	C	454	GLN	C-N-CA	6.96	129.50	120.44
2	D	200	ASP	N-CA-CB	-6.96	102.39	111.23
2	D	608	GLU	CA-C-O	-6.96	113.51	120.82
2	D	87	TYR	CB-CG-CD1	6.96	131.24	120.80
2	B	611	LYS	CA-C-O	-6.96	112.24	120.10
1	C	383	ALA	O-C-N	-6.96	114.08	122.22
1	A	572	LYS	CB-CA-C	-6.96	99.68	110.81
2	D	35	TRP	O-C-N	-6.96	114.80	122.03
1	A	112	GLY	O-C-N	-6.95	117.25	123.37
2	B	62	LEU	CA-C-N	6.95	131.68	122.30
2	B	62	LEU	C-N-CA	6.95	131.68	122.30
1	C	26	GLU	O-C-N	-6.95	113.35	122.59
2	D	73	VAL	CA-C-N	6.95	126.55	119.19
2	D	73	VAL	C-N-CA	6.95	126.55	119.19
2	B	282	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	688	ILE	O-C-N	6.94	127.39	120.59
2	B	629	SER	CA-C-O	-6.94	113.44	121.07
2	B	633	ILE	CA-C-N	6.94	135.82	121.94
2	B	633	ILE	C-N-CA	6.94	135.82	121.94
1	C	723	ARG	NE-CZ-NH1	6.94	128.44	121.50
1	A	228	THR	CA-C-O	-6.94	113.54	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	THR	CA-CB-CG2	6.93	122.29	110.50
2	D	425	LYS	CB-CG-CD	6.93	127.25	111.30
2	D	566	ASP	CA-CB-CG	6.93	119.53	112.60
1	C	145	SER	CA-C-N	6.93	131.42	120.47
1	C	145	SER	C-N-CA	6.93	131.42	120.47
1	A	667	ALA	O-C-N	-6.93	114.12	122.22
1	A	503	ARG	CD-NE-CZ	6.92	134.09	124.40
2	B	130	GLU	CA-C-N	6.91	134.75	121.54
2	B	130	GLU	C-N-CA	6.91	134.75	121.54
1	C	163	VAL	CA-C-O	6.91	127.65	120.39
1	C	366	ASN	CA-C-N	6.91	134.39	122.64
1	C	366	ASN	C-N-CA	6.91	134.39	122.64
2	B	29	LYS	CA-C-O	-6.91	112.75	120.70
2	D	157	VAL	CB-CA-C	-6.91	103.00	111.08
1	A	518	ALA	O-C-N	-6.91	114.80	122.12
1	A	622	ALA	CA-C-N	6.91	131.65	120.60
1	A	622	ALA	C-N-CA	6.91	131.65	120.60
1	C	227	TYR	CA-C-N	6.91	129.42	120.44
1	C	227	TYR	C-N-CA	6.91	129.42	120.44
2	D	429	MET	O-C-N	-6.91	114.80	122.12
1	A	699	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	714	SER	O-C-N	-6.91	114.14	122.22
1	C	131	ARG	N-CA-C	6.91	120.59	111.75
2	D	501	MET	CA-CB-CG	6.90	127.91	114.10
1	C	118	ASP	CA-CB-CG	6.90	119.50	112.60
1	C	462	GLN	OE1-CD-NE2	6.90	129.50	122.60
1	A	452	ARG	CD-NE-CZ	6.90	134.06	124.40
1	A	292	MET	O-C-N	-6.90	113.79	122.27
2	D	218	GLY	O-C-N	-6.89	113.74	122.70
2	B	550	THR	N-CA-CB	6.89	119.97	109.91
1	C	703	GLU	CA-CB-CG	6.89	127.88	114.10
2	B	298	ARG	CG-CD-NE	6.89	127.15	112.00
1	C	158	LEU	N-CA-C	6.88	120.78	112.38
1	C	462	GLN	CA-C-O	6.88	123.77	119.29
2	D	555	GLU	N-CA-CB	6.88	119.98	110.01
2	B	293	THR	O-C-N	-6.87	114.99	122.07
1	C	246	GLN	N-CA-C	-6.87	103.72	111.07
1	C	554	LYS	CA-C-O	-6.87	113.51	121.07
2	D	47	ARG	CA-C-O	6.87	127.30	119.61
2	B	351	SER	O-C-N	-6.87	114.84	122.12
2	B	445	CYS	CA-C-N	6.87	130.75	120.31
2	B	445	CYS	C-N-CA	6.87	130.75	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	PRO	N-CA-CB	6.87	110.63	103.15
2	D	414	ASP	O-C-N	-6.87	114.84	122.12
1	A	561	ALA	CA-C-O	-6.86	113.62	121.72
1	A	673	ASP	O-C-N	-6.86	114.33	122.15
2	D	423	VAL	CA-C-N	6.86	129.36	120.44
2	D	423	VAL	C-N-CA	6.86	129.36	120.44
2	D	100	ARG	CA-C-O	-6.85	113.19	120.80
1	A	219	ARG	NE-CZ-NH2	-6.84	113.04	119.20
2	B	515	LEU	O-C-N	-6.84	115.20	123.27
1	C	449	ALA	O-C-N	-6.84	114.98	122.09
1	A	347	ARG	O-C-N	-6.84	114.87	122.12
2	D	23	LEU	O-C-N	-6.83	115.09	121.79
1	C	509	LYS	CA-C-N	6.83	129.67	120.65
1	C	509	LYS	C-N-CA	6.83	129.67	120.65
1	C	548	MET	O-C-N	-6.83	114.88	122.12
2	B	378	ILE	CA-C-N	6.83	129.76	120.54
2	B	378	ILE	C-N-CA	6.83	129.76	120.54
1	C	598	PRO	N-CA-C	-6.83	100.47	111.19
1	A	459	SER	O-C-N	-6.83	113.04	122.46
1	C	337	THR	CA-CB-CG2	6.83	122.11	110.50
1	C	328	HIS	N-CA-C	-6.82	99.84	110.42
1	C	704	ILE	CA-C-N	6.82	133.43	123.13
1	C	704	ILE	C-N-CA	6.82	133.43	123.13
2	D	107	TRP	CA-C-N	-6.82	113.70	122.77
2	D	107	TRP	C-N-CA	-6.82	113.70	122.77
2	D	141	ASP	CA-C-N	6.82	126.78	119.28
2	D	141	ASP	C-N-CA	6.82	126.78	119.28
2	B	600	LYS	O-C-N	-6.81	114.25	122.22
2	D	501	MET	O-C-N	-6.81	115.05	122.07
2	B	417	TRP	O-C-N	-6.81	114.95	122.03
1	C	558	ARG	NE-CZ-NH2	-6.81	113.07	119.20
1	A	554	LYS	N-CA-CB	6.81	120.09	109.94
2	B	229	PRO	CA-C-O	6.81	128.26	118.86
2	D	572	LYS	CA-C-O	-6.81	113.67	120.82
2	B	64	VAL	CA-CB-CG1	6.81	121.97	110.40
1	A	221	ILE	N-CA-CB	6.80	117.77	110.62
1	C	222	SER	O-C-N	-6.80	114.44	122.20
2	B	46	GLY	N-CA-C	6.80	125.09	115.30
1	C	4	LEU	CA-C-N	6.80	126.82	119.89
1	C	4	LEU	C-N-CA	6.80	126.82	119.89
1	C	703	GLU	O-C-N	-6.80	115.11	123.33
1	A	469	LYS	CA-C-N	6.79	132.27	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LYS	C-N-CA	6.79	132.27	122.35
2	B	292	LEU	N-CA-C	-6.79	103.95	111.36
1	C	576	ASN	N-CA-C	6.79	120.91	111.74
2	B	365	GLN	N-CA-C	6.79	121.17	112.34
2	B	463	VAL	O-C-N	6.79	131.06	122.57
1	A	369	ASP	O-C-N	-6.79	113.00	122.37
1	C	10	VAL	CA-C-O	-6.79	113.97	121.23
1	C	150	ARG	CB-CA-C	-6.79	100.23	110.88
1	A	193	ALA	CA-C-N	-6.78	111.55	120.91
1	A	193	ALA	C-N-CA	-6.78	111.55	120.91
2	B	121	THR	CA-CB-OG1	-6.78	99.43	109.60
1	C	219	ARG	CD-NE-CZ	-6.78	114.92	124.40
2	D	528	GLU	CA-C-N	6.77	128.82	120.22
2	D	528	GLU	C-N-CA	6.77	128.82	120.22
1	A	27	GLU	CB-CG-CD	6.77	124.11	112.60
1	A	271	GLU	CA-C-N	6.77	130.03	120.28
1	A	271	GLU	C-N-CA	6.77	130.03	120.28
2	B	411	SER	CA-CB-OG	-6.77	97.56	111.10
2	D	306	ARG	N-CA-CB	6.77	119.80	109.91
2	D	337	TYR	CA-C-N	6.77	131.17	120.47
2	D	337	TYR	C-N-CA	6.77	131.17	120.47
2	D	536	HIS	O-C-N	-6.77	113.59	122.39
2	D	336	PRO	N-CA-CB	6.77	110.77	103.33
1	C	360	THR	O-C-N	-6.77	114.88	122.86
2	D	341	LEU	CA-C-O	-6.76	113.25	120.42
1	A	539	GLY	CA-C-N	6.76	129.67	120.54
1	A	539	GLY	C-N-CA	6.76	129.67	120.54
1	C	554	LYS	N-CA-CB	6.76	120.10	109.82
1	A	430	VAL	CA-CB-CG1	6.76	121.89	110.40
2	B	557	PHE	CA-C-N	6.76	129.23	120.44
2	B	557	PHE	C-N-CA	6.76	129.23	120.44
1	A	633	LEU	CA-C-N	6.76	133.66	123.05
1	A	633	LEU	C-N-CA	6.76	133.66	123.05
1	C	322	SER	O-C-N	-6.76	114.50	122.20
1	C	388	LEU	CA-C-N	6.76	130.18	120.79
1	C	388	LEU	C-N-CA	6.76	130.18	120.79
1	C	229	SER	O-C-N	-6.75	114.96	122.12
1	A	353	MET	CA-C-N	6.75	129.22	120.44
1	A	353	MET	C-N-CA	6.75	129.22	120.44
2	B	427	GLY	CA-C-N	-6.75	113.58	122.63
2	B	427	GLY	C-N-CA	-6.75	113.58	122.63
1	C	55	TYR	N-CA-C	6.75	119.21	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	LEU	N-CA-C	-6.75	103.61	110.97
1	A	95	ALA	O-C-N	-6.75	114.97	122.12
2	D	424	GLU	CA-C-N	6.75	131.40	120.60
2	D	424	GLU	C-N-CA	6.75	131.40	120.60
1	A	698	LYS	N-CA-C	6.75	119.47	111.71
1	A	675	LEU	CA-C-N	6.74	132.93	120.87
1	A	675	LEU	C-N-CA	6.74	132.93	120.87
1	C	313	HIS	O-C-N	-6.74	115.13	122.07
2	D	613	ILE	CA-C-N	6.74	134.59	122.06
2	D	613	ILE	C-N-CA	6.74	134.59	122.06
2	B	218	GLY	O-C-N	-6.73	115.64	122.17
1	C	246	GLN	N-CA-CB	6.73	119.77	110.01
1	A	574	VAL	CA-CB-CG2	6.73	121.84	110.40
1	C	39	GLU	CB-CA-C	6.72	120.85	109.75
1	A	149	MET	O-C-N	-6.72	115.00	122.12
2	D	348	PHE	CA-CB-CG	6.72	120.52	113.80
2	D	355	ALA	CA-C-O	6.72	128.54	121.15
2	D	510	ARG	NH1-CZ-NH2	-6.72	110.57	119.30
2	D	612	LEU	O-C-N	-6.72	114.01	122.27
1	C	638	GLU	CA-C-O	-6.72	113.30	120.42
1	A	266	TYR	CA-C-O	-6.71	112.25	119.97
1	C	430	VAL	N-CA-CB	-6.71	100.15	111.23
1	A	597	ARG	NE-CZ-NH1	6.71	128.21	121.50
1	A	385	ASN	CA-C-O	-6.71	113.44	120.55
1	C	274	GLY	N-CA-C	6.71	124.04	114.64
2	D	221	VAL	CB-CA-C	-6.71	103.29	111.88
1	C	157	PRO	N-CA-CB	6.71	110.29	103.25
1	C	222	SER	CA-C-N	6.70	132.07	120.68
1	C	222	SER	C-N-CA	6.70	132.07	120.68
1	A	553	GLU	CA-C-N	6.70	129.58	120.54
1	A	553	GLU	C-N-CA	6.70	129.58	120.54
1	A	639	GLU	CA-C-N	6.70	129.80	120.29
1	A	639	GLU	C-N-CA	6.70	129.80	120.29
1	A	686	GLY	N-CA-C	6.70	118.33	111.56
1	C	105	ASN	CA-C-N	6.70	129.49	120.65
1	C	105	ASN	C-N-CA	6.70	129.49	120.65
1	C	460	GLY	CA-C-O	6.70	126.03	118.86
1	A	171	VAL	CB-CA-C	6.69	120.27	111.70
2	B	636	VAL	CB-CA-C	6.69	120.42	110.98
1	C	271	GLU	N-CA-C	-6.69	103.91	111.14
2	D	483	PRO	CB-CA-C	-6.69	102.83	111.46
2	B	604	ASP	O-C-N	-6.69	113.53	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	594	GLU	CB-CA-C	6.69	121.29	109.65
1	A	189	PRO	O-C-N	-6.69	114.55	122.24
1	A	282	PRO	CA-C-N	6.69	132.67	122.37
1	A	282	PRO	C-N-CA	6.69	132.67	122.37
1	A	457	ILE	CA-C-N	6.68	129.54	120.38
1	A	457	ILE	C-N-CA	6.68	129.54	120.38
1	C	251	THR	N-CA-C	-6.68	100.91	110.59
2	D	77	ARG	O-C-N	-6.68	113.64	121.32
1	A	143	ILE	O-C-N	-6.67	116.05	123.26
2	D	507	VAL	CA-C-O	6.67	129.05	121.11
1	A	405	GLY	CA-C-O	-6.67	108.97	120.57
1	C	111	LYS	CB-CG-CD	6.67	126.64	111.30
2	D	78	PRO	CA-C-N	6.67	130.82	120.82
2	D	78	PRO	C-N-CA	6.67	130.82	120.82
1	A	646	GLU	O-C-N	-6.66	113.67	122.33
1	C	23	ARG	O-C-N	-6.66	114.43	122.22
2	D	456	ARG	CA-C-N	6.66	134.44	122.38
2	D	456	ARG	C-N-CA	6.66	134.44	122.38
1	A	55	TYR	CA-C-N	6.66	134.26	121.54
1	A	55	TYR	C-N-CA	6.66	134.26	121.54
1	A	410	GLU	CA-C-O	-6.66	113.83	120.82
1	A	421	TRP	O-C-N	-6.66	114.43	122.22
1	A	616	VAL	CB-CA-C	6.65	120.76	112.04
1	C	649	VAL	CA-C-O	-6.65	113.93	121.98
2	B	67	VAL	N-CA-CB	-6.65	100.09	110.54
1	A	85	THR	O-C-N	-6.65	115.26	123.04
1	A	206	VAL	CB-CA-C	-6.65	100.39	111.29
2	B	404	TYR	CA-CB-CG	6.65	125.86	113.90
2	D	146	ALA	CA-C-O	6.64	127.01	120.23
1	A	425	GLN	O-C-N	-6.64	115.23	122.07
1	C	397	THR	CA-C-N	6.64	129.47	120.38
1	C	397	THR	C-N-CA	6.64	129.47	120.38
2	B	424	GLU	CB-CG-CD	6.64	123.88	112.60
2	D	245	GLY	CA-C-N	-6.64	110.52	120.94
2	D	245	GLY	C-N-CA	-6.64	110.52	120.94
1	C	267	ILE	N-CA-CB	6.63	118.14	110.65
1	A	661	HIS	CA-CB-CG	-6.63	107.17	113.80
1	C	207	ARG	CG-CD-NE	6.63	126.58	112.00
2	D	369	LEU	CA-C-O	6.63	126.35	120.19
1	A	188	LYS	CA-C-N	6.63	126.88	119.32
1	A	188	LYS	C-N-CA	6.63	126.88	119.32
1	A	310	LYS	O-C-N	-6.63	114.93	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	522	ARG	CA-C-N	6.63	136.11	121.80
2	B	522	ARG	C-N-CA	6.63	136.11	121.80
1	C	5	PRO	N-CA-CB	6.63	108.89	103.32
1	C	305	ARG	CA-C-O	-6.63	113.86	120.82
1	A	232	MET	CA-C-N	6.62	126.25	119.56
1	A	232	MET	C-N-CA	6.62	126.25	119.56
1	A	381	ARG	O-C-N	-6.62	115.25	122.07
1	C	327	THR	N-CA-CB	-6.62	99.75	111.08
2	D	31	THR	CA-C-N	6.62	129.16	120.28
2	D	31	THR	C-N-CA	6.62	129.16	120.28
2	D	417	TRP	O-C-N	-6.62	114.88	122.03
2	B	342	ARG	CB-CG-CD	6.62	126.53	111.30
1	A	291	GLY	O-C-N	-6.62	116.41	122.96
1	C	588	GLU	CA-C-O	-6.62	113.87	120.82
2	D	142	PRO	CA-C-N	6.62	133.71	122.26
2	D	142	PRO	C-N-CA	6.62	133.71	122.26
1	A	642	ARG	CA-C-O	-6.62	113.82	120.90
2	B	528	GLU	O-C-N	-6.62	114.61	122.15
2	B	363	PHE	CA-CB-CG	6.61	120.41	113.80
2	D	360	THR	N-CA-CB	-6.61	100.17	110.55
1	C	319	ASN	N-CA-C	-6.60	100.04	109.62
2	D	422	GLU	O-C-N	-6.60	114.52	122.11
1	C	269	ALA	O-C-N	-6.60	115.02	122.08
2	D	278	ASP	O-C-N	-6.60	113.65	122.43
2	D	585	LEU	CB-CA-C	6.60	121.42	110.92
1	C	437	ILE	O-C-N	-6.60	114.34	121.80
1	A	146	ILE	O-C-N	-6.60	115.34	121.94
1	A	402	PRO	CA-C-N	6.60	134.44	121.58
1	A	402	PRO	C-N-CA	6.60	134.44	121.58
2	D	332	THR	O-C-N	6.59	131.35	123.24
1	A	215	GLN	CA-C-O	6.59	129.19	120.16
1	C	601	LEU	N-CA-C	-6.59	97.99	108.73
2	B	308	GLY	CA-C-N	6.59	131.71	120.71
2	B	308	GLY	C-N-CA	6.59	131.71	120.71
2	D	441	VAL	CA-C-O	6.58	128.36	121.05
1	C	637	PRO	CA-C-N	6.58	129.63	120.29
1	C	637	PRO	C-N-CA	6.58	129.63	120.29
1	A	628	VAL	N-CA-C	6.58	117.77	108.36
2	B	425	LYS	O-C-N	-6.58	115.15	122.12
2	B	381	ASN	CB-CA-C	6.57	122.79	110.63
2	B	507	VAL	CA-C-N	6.57	131.69	120.72
2	B	507	VAL	C-N-CA	6.57	131.69	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	254	TRP	CA-C-N	6.57	129.32	120.65
2	D	254	TRP	C-N-CA	6.57	129.32	120.65
2	B	622	ASP	N-CA-C	-6.57	98.52	108.96
1	C	564	ARG	O-C-N	-6.57	114.88	123.28
2	D	305	ALA	O-C-N	-6.56	115.16	122.12
1	A	656	SER	O-C-N	-6.56	115.55	123.29
1	C	592	GLN	CB-CA-C	-6.56	99.70	110.85
2	D	135	SER	CA-C-O	-6.56	114.12	121.40
1	A	276	ASN	N-CA-C	-6.56	99.89	110.32
1	C	507	LYS	CA-C-N	6.56	129.36	120.77
1	C	507	LYS	C-N-CA	6.56	129.36	120.77
1	A	368	LEU	N-CA-C	6.55	120.54	112.54
2	B	523	ASP	O-C-N	6.55	131.15	122.30
2	B	554	VAL	N-CA-C	6.55	117.24	110.36
1	A	217	SER	CA-C-N	6.55	129.06	120.28
1	A	217	SER	C-N-CA	6.55	129.06	120.28
1	C	79	TYR	O-C-N	-6.54	113.66	122.43
2	B	361	LEU	CA-C-N	6.54	126.92	119.92
2	B	361	LEU	C-N-CA	6.54	126.92	119.92
1	A	523	ASP	N-CA-CB	6.54	122.26	110.95
2	B	187	ASP	O-C-N	-6.54	113.30	122.06
1	C	15	ALA	CA-C-O	6.54	129.11	120.16
2	D	610	GLU	O-C-N	-6.54	115.19	122.12
2	D	359	THR	CA-C-N	-6.53	113.90	123.05
2	D	359	THR	C-N-CA	-6.53	113.90	123.05
2	B	541	ASP	N-CA-CB	6.53	119.70	110.36
1	C	252	ALA	CA-C-N	6.53	131.78	120.68
1	C	252	ALA	C-N-CA	6.53	131.78	120.68
2	D	228	SER	CA-CB-OG	6.53	124.16	111.10
2	D	33	GLU	O-C-N	-6.53	115.30	122.09
2	D	214	LEU	CA-C-N	6.53	129.56	120.29
2	D	214	LEU	C-N-CA	6.53	129.56	120.29
2	D	225	ALA	CA-C-N	6.52	129.86	120.79
2	D	225	ALA	C-N-CA	6.52	129.86	120.79
2	B	213	ASP	CA-CB-CG	6.52	119.12	112.60
2	D	229	PRO	CA-C-O	6.52	128.13	119.00
2	D	296	ARG	CA-C-O	-6.52	113.98	120.70
2	B	417	TRP	CA-C-N	6.52	128.91	120.44
2	B	417	TRP	C-N-CA	6.52	128.91	120.44
1	C	319	ASN	CA-C-O	6.52	126.91	119.61
2	D	403	TYR	CB-CG-CD1	6.52	130.57	120.80
1	A	477	PRO	N-CA-CB	6.51	108.98	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	LEU	N-CA-C	6.51	119.20	111.71
1	C	575	LYS	O-C-N	-6.51	115.37	122.79
2	D	574	TYR	CA-C-O	6.51	127.66	120.63
2	B	450	ALA	CA-C-N	6.51	129.29	120.44
2	B	450	ALA	C-N-CA	6.51	129.29	120.44
2	D	411	SER	N-CA-C	6.50	119.19	111.71
1	C	528	ASP	CA-CB-CG	6.50	119.10	112.60
2	B	507	VAL	N-CA-CB	-6.50	97.78	110.45
2	B	196	ASN	CA-CB-CG	6.50	119.09	112.60
2	D	283	ARG	CB-CG-CD	6.50	126.24	111.30
1	A	19	ALA	O-C-N	-6.49	115.24	122.12
2	B	68	ASP	CA-CB-CG	6.49	119.09	112.60
2	D	169	ARG	CA-CB-CG	6.49	127.08	114.10
2	D	142	PRO	N-CA-C	6.49	122.41	113.65
1	A	277	VAL	CA-C-N	6.49	133.06	120.99
1	A	277	VAL	C-N-CA	6.49	133.06	120.99
1	A	723	ARG	NE-CZ-NH1	6.48	127.98	121.50
1	A	577	THR	N-CA-CB	-6.48	102.19	110.03
1	C	53	ASP	CA-CB-CG	6.48	119.08	112.60
2	D	158	LEU	CA-C-N	6.48	129.84	120.38
2	D	158	LEU	C-N-CA	6.48	129.84	120.38
2	B	205	ALA	CA-C-N	6.47	129.28	120.54
2	B	205	ALA	C-N-CA	6.47	129.28	120.54
2	D	472	ARG	CD-NE-CZ	6.47	133.46	124.40
1	C	359	HIS	ND1-CE1-NE2	6.47	114.87	108.40
2	D	413	ALA	CA-C-N	6.47	128.95	120.28
2	D	413	ALA	C-N-CA	6.47	128.95	120.28
2	D	531	SER	O-C-N	-6.47	115.30	122.03
2	B	418	LYS	O-C-N	-6.46	115.41	122.07
2	D	360	THR	CB-CA-C	6.46	120.79	110.19
1	A	623	ASP	CA-C-N	6.46	133.44	122.26
1	A	623	ASP	C-N-CA	6.46	133.44	122.26
1	C	69	PRO	CA-C-N	6.46	133.88	121.54
1	C	69	PRO	C-N-CA	6.46	133.88	121.54
1	A	596	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	C	357	GLN	O-C-N	-6.46	113.78	122.43
2	B	288	HIS	CA-CB-CG	6.46	120.25	113.80
2	B	553	ILE	CA-C-N	6.46	128.93	120.60
2	B	553	ILE	C-N-CA	6.46	128.93	120.60
1	C	509	LYS	O-C-N	-6.45	114.67	122.22
2	D	328	TRP	CA-C-O	6.45	127.40	120.24
2	B	21	LEU	CA-C-O	6.45	128.27	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	613	ILE	CA-C-O	6.45	127.99	120.71
1	C	150	ARG	CD-NE-CZ	6.44	133.42	124.40
2	D	132	GLY	N-CA-C	6.44	123.91	115.40
1	C	190	GLU	CA-C-N	6.44	134.04	122.06
1	C	190	GLU	C-N-CA	6.44	134.04	122.06
1	C	671	GLU	N-CA-C	6.44	119.13	111.33
2	D	421	GLN	CG-CD-OE1	6.44	133.68	120.80
1	A	507	LYS	CA-C-N	6.44	129.20	120.77
1	A	507	LYS	C-N-CA	6.44	129.20	120.77
1	C	264	VAL	CA-C-O	-6.44	114.35	121.17
1	C	363	LEU	N-CA-CB	-6.44	99.55	111.52
1	A	80	ALA	CA-C-N	6.44	134.89	122.53
1	A	80	ALA	C-N-CA	6.44	134.89	122.53
1	A	502	GLU	N-CA-C	6.43	119.28	111.82
2	B	521	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	A	248	ALA	CA-C-N	6.43	134.02	121.41
1	A	248	ALA	C-N-CA	6.43	134.02	121.41
2	B	357	SER	O-C-N	-6.43	115.92	123.25
2	D	286	ALA	N-CA-CB	6.43	120.68	110.65
1	A	242	GLY	O-C-N	-6.43	114.34	122.70
2	B	335	ASP	CA-C-N	6.43	126.35	119.28
2	B	335	ASP	C-N-CA	6.43	126.35	119.28
2	B	283	ARG	N-CA-CB	6.43	120.98	110.37
1	A	183	GLU	O-C-N	-6.42	115.41	122.09
2	B	482	ALA	CA-C-N	6.42	126.38	119.76
2	B	482	ALA	C-N-CA	6.42	126.38	119.76
1	C	586	LEU	O-C-N	-6.42	114.88	122.20
1	A	621	TYR	CA-C-N	6.42	128.79	120.44
1	A	621	TYR	C-N-CA	6.42	128.79	120.44
1	A	314	GLN	O-C-N	-6.42	114.83	122.15
2	B	48	PRO	CA-C-N	6.42	127.86	119.84
2	B	48	PRO	C-N-CA	6.42	127.86	119.84
2	D	77	ARG	CA-C-N	6.42	125.92	119.24
2	D	77	ARG	C-N-CA	6.42	125.92	119.24
2	D	212	PRO	N-CA-CB	6.42	108.44	103.30
2	B	413	ALA	N-CA-C	-6.42	103.98	110.97
1	C	423	HIS	CA-CB-CG	6.42	120.22	113.80
1	A	658	ALA	N-CA-C	6.42	120.81	112.92
1	C	722	LEU	N-CA-C	-6.42	103.98	110.97
1	C	619	THR	O-C-N	-6.41	115.32	122.12
2	D	57	GLU	CA-C-O	-6.41	114.09	120.70
1	A	342	TYR	CA-C-N	6.41	129.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TYR	C-N-CA	6.41	129.51	120.28
1	A	575	LYS	CA-C-N	6.41	131.97	122.74
1	A	575	LYS	C-N-CA	6.41	131.97	122.74
2	B	328	TRP	CA-C-N	6.41	129.19	120.54
2	B	328	TRP	C-N-CA	6.41	129.19	120.54
2	D	455	ASN	CA-C-O	6.41	127.06	119.56
2	B	100	ARG	NH1-CZ-NH2	6.41	127.63	119.30
2	B	559	LYS	O-C-N	-6.41	115.33	122.12
1	C	177	LEU	CA-C-N	6.41	128.77	120.44
1	C	177	LEU	C-N-CA	6.41	128.77	120.44
1	C	666	PRO	CA-C-N	6.41	129.39	120.29
1	C	666	PRO	C-N-CA	6.41	129.39	120.29
1	A	189	PRO	CA-C-N	6.41	131.42	120.72
1	A	189	PRO	C-N-CA	6.41	131.42	120.72
1	A	349	CYS	O-C-N	-6.41	115.22	122.08
1	A	589	GLU	O-C-N	-6.41	115.33	122.12
1	C	661	HIS	O-C-N	-6.41	114.07	122.59
1	C	409	VAL	N-CA-CB	6.40	118.04	110.55
1	C	688	ILE	O-C-N	6.40	126.86	120.59
1	A	121	THR	O-C-N	-6.40	115.48	122.07
1	A	267	ILE	O-C-N	-6.40	115.64	121.91
2	D	199	LEU	CA-C-N	-6.40	116.65	122.28
2	D	199	LEU	C-N-CA	-6.40	116.65	122.28
1	A	345	VAL	CA-C-O	-6.40	114.39	121.17
2	B	408	LEU	CA-C-N	6.40	128.76	120.44
2	B	408	LEU	C-N-CA	6.40	128.76	120.44
2	D	66	THR	O-C-N	-6.39	114.79	122.65
2	B	62	LEU	O-C-N	-6.39	114.15	122.39
1	A	332	SER	N-CA-C	6.39	118.35	109.15
1	A	145	SER	CA-C-O	6.38	127.75	121.05
2	B	228	SER	CA-C-O	6.38	128.91	120.16
1	C	88	GLN	OE1-CD-NE2	6.38	128.99	122.60
1	A	617	ILE	CA-C-N	6.37	129.65	120.79
1	A	617	ILE	C-N-CA	6.37	129.65	120.79
2	B	27	PHE	CA-C-O	6.37	127.22	120.66
1	C	375	PRO	N-CA-CB	6.37	108.86	103.25
1	A	453	THR	CA-C-O	-6.37	114.13	120.82
2	B	552	GLU	CA-C-O	-6.36	113.81	120.55
2	D	499	GLN	N-CA-C	-6.36	104.26	111.07
1	A	70	PHE	O-C-N	-6.36	114.07	122.40
1	C	115	VAL	CB-CA-C	-6.36	102.88	111.15
1	C	70	PHE	CA-C-O	6.36	129.60	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	ASP	N-CA-CB	6.36	121.09	110.41
2	D	348	PHE	CA-C-N	6.36	129.12	120.54
2	D	348	PHE	C-N-CA	6.36	129.12	120.54
1	A	723	ARG	CA-C-N	6.35	129.65	120.38
1	A	723	ARG	C-N-CA	6.35	129.65	120.38
1	C	563	ILE	O-C-N	-6.35	115.69	122.61
2	D	159	LEU	CA-C-N	6.35	129.31	120.29
2	D	159	LEU	C-N-CA	6.35	129.31	120.29
2	D	575	ALA	N-CA-C	-6.35	104.27	111.07
2	B	526	GLY	O-C-N	-6.35	114.44	122.70
1	C	521	ASN	CB-CA-C	-6.35	100.84	110.87
1	C	266	TYR	O-C-N	-6.35	114.14	122.39
2	D	513	VAL	O-C-N	-6.35	117.26	122.97
2	B	223	ARG	CG-CD-NE	6.34	125.96	112.00
1	A	150	ARG	CB-CA-C	-6.34	100.26	110.79
1	A	400	ILE	CA-C-N	6.34	137.27	121.80
1	A	400	ILE	C-N-CA	6.34	137.27	121.80
1	C	723	ARG	O-C-N	-6.34	114.53	122.20
1	C	707	PRO	N-CA-CB	6.34	108.83	103.25
2	B	261	GLU	N-CA-CB	6.34	119.20	110.01
2	B	100	ARG	CD-NE-CZ	6.33	133.27	124.40
1	A	131	ARG	O-C-N	-6.33	113.94	122.43
1	A	276	ASN	CA-CB-CG	6.33	118.93	112.60
2	B	154	LEU	O-C-N	-6.33	113.18	122.43
1	C	490	ALA	CA-C-O	-6.33	114.17	120.82
2	D	108	ASP	CB-CA-C	6.33	120.45	110.19
2	D	577	GLN	N-CA-C	6.33	121.05	112.88
1	C	103	ARG	CA-CB-CG	-6.33	101.44	114.10
2	D	540	ILE	N-CA-CB	-6.33	104.05	111.39
1	C	275	LEU	N-CA-C	6.33	119.82	109.76
1	C	505	PRO	N-CA-CB	6.33	110.23	103.52
2	B	224	LEU	N-CA-CB	-6.33	100.76	110.44
1	A	72	HIS	N-CA-C	6.32	120.71	113.19
1	A	188	LYS	CA-C-O	6.32	127.15	120.64
1	A	607	GLN	CA-C-N	6.32	131.31	121.26
1	A	607	GLN	C-N-CA	6.32	131.31	121.26
1	C	359	HIS	CA-C-O	6.32	129.55	120.51
2	D	29	LYS	N-CA-CB	6.32	119.27	109.85
1	C	88	GLN	CA-C-N	6.32	129.80	120.95
1	C	88	GLN	C-N-CA	6.32	129.80	120.95
2	D	347	THR	CA-C-O	6.32	127.66	120.90
2	B	228	SER	CA-CB-OG	6.32	123.73	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	720	LYS	CA-C-N	6.32	129.03	120.44
1	C	720	LYS	C-N-CA	6.32	129.03	120.44
2	D	188	LYS	CB-CA-C	6.32	118.38	108.84
1	C	23	ARG	CA-C-N	6.31	129.90	120.31
1	C	23	ARG	C-N-CA	6.31	129.90	120.31
1	C	614	GLN	OE1-CD-NE2	-6.31	116.29	122.60
2	B	27	PHE	CA-C-N	6.31	126.25	119.76
2	B	27	PHE	C-N-CA	6.31	126.25	119.76
1	A	256	MET	CG-SD-CE	-6.30	87.03	100.90
2	D	347	THR	CA-C-N	6.30	128.64	120.44
2	D	347	THR	C-N-CA	6.30	128.64	120.44
1	A	158	LEU	O-C-N	-6.30	114.05	122.43
1	A	272	SER	CA-C-O	-6.30	112.98	120.10
2	B	631	LEU	CA-C-O	-6.30	113.74	120.42
2	D	424	GLU	O-C-N	-6.30	115.58	122.07
2	B	401	GLY	O-C-N	-6.30	114.51	122.70
1	C	217	SER	CA-C-N	6.30	128.72	120.28
1	C	217	SER	C-N-CA	6.30	128.72	120.28
2	D	379	ALA	CA-C-O	-6.30	114.14	121.07
2	B	227	PHE	CA-CB-CG	6.29	120.09	113.80
2	D	281	ASN	CA-CB-CG	6.29	118.89	112.60
1	C	634	PHE	N-CA-CB	-6.29	102.66	112.41
1	C	639	GLU	CA-C-O	6.29	127.20	119.97
1	C	551	ALA	CA-C-N	6.29	132.73	121.66
1	C	551	ALA	C-N-CA	6.29	132.73	121.66
1	C	677	ARG	CA-C-O	6.29	127.61	121.32
1	C	202	LYS	CA-C-N	6.29	128.99	120.44
1	C	202	LYS	C-N-CA	6.29	128.99	120.44
2	D	169	ARG	N-CA-C	-6.29	103.96	113.89
1	C	599	ARG	N-CA-CB	-6.28	99.93	110.80
1	C	222	SER	N-CA-C	6.28	119.79	111.75
2	D	31	THR	O-C-N	-6.28	115.93	123.03
2	D	93	PHE	CA-C-O	6.28	129.12	118.94
1	A	134	GLY	CA-C-O	-6.28	112.09	119.50
2	B	344	SER	O-C-N	-6.28	115.36	122.08
2	D	319	GLY	O-C-N	6.28	128.30	122.77
1	C	167	MET	CA-C-O	6.28	128.68	120.21
2	D	242	HIS	N-CA-C	-6.28	104.36	111.14
1	A	498	LYS	O-C-N	-6.27	114.61	122.20
1	A	582	GLU	CB-CG-CD	6.27	123.26	112.60
2	D	328	TRP	N-CA-C	-6.27	103.98	111.69
2	B	409	THR	CA-C-N	6.27	128.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	409	THR	C-N-CA	6.27	128.68	120.28
2	B	509	GLU	CA-C-O	-6.27	113.59	120.24
1	A	24	ARG	CA-C-N	6.26	128.59	120.44
1	A	24	ARG	C-N-CA	6.26	128.59	120.44
1	A	689	PRO	CB-CA-C	-6.26	103.38	111.46
2	B	449	ARG	CD-NE-CZ	6.26	133.17	124.40
2	B	544	GLN	CA-CB-CG	6.26	126.63	114.10
1	A	387	GLN	O-C-N	-6.26	115.01	122.15
1	A	8	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	219	ARG	NE-CZ-NH1	-6.26	115.24	121.50
2	D	55	PHE	O-C-N	-6.26	115.48	122.12
1	C	67	ILE	CA-C-N	6.26	126.83	120.38
1	C	67	ILE	C-N-CA	6.26	126.83	120.38
1	C	535	CYS	O-C-N	-6.26	114.04	122.43
1	C	694	ASP	CB-CA-C	6.26	122.15	110.70
2	D	141	ASP	O-C-N	-6.26	114.12	121.32
1	A	121	THR	CA-C-O	-6.25	114.25	120.82
2	D	145	ILE	CA-CB-CG2	6.25	121.13	110.50
1	A	532	LEU	CA-C-O	6.25	127.05	120.42
1	C	313	HIS	CA-CB-CG	-6.25	107.55	113.80
2	B	555	GLU	CB-CG-CD	6.25	123.22	112.60
1	C	64	TYR	N-CA-C	6.25	119.65	109.59
1	C	151	GLU	O-C-N	-6.25	115.63	122.07
1	C	326	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	C	578	PRO	N-CA-CB	6.25	109.92	103.23
1	C	600	ILE	N-CA-C	6.25	117.48	108.48
1	A	105	ASN	CA-C-N	6.25	128.56	120.44
1	A	105	ASN	C-N-CA	6.25	128.56	120.44
2	D	429	MET	CB-CG-SD	6.25	131.44	112.70
2	D	482	ALA	CA-C-N	6.25	126.19	119.76
2	D	482	ALA	C-N-CA	6.25	126.19	119.76
2	B	443	ASP	CA-CB-CG	6.25	118.84	112.60
1	C	429	LYS	CA-C-N	6.24	133.20	121.97
1	C	429	LYS	C-N-CA	6.24	133.20	121.97
1	C	678	PRO	O-C-N	-6.24	112.36	122.47
2	B	475	GLU	CA-C-O	-6.24	114.33	121.19
2	D	269	GLN	CB-CG-CD	6.24	123.20	112.60
1	A	719	VAL	CA-C-N	6.24	128.96	120.54
1	A	719	VAL	C-N-CA	6.24	128.96	120.54
1	A	33	GLY	CA-C-N	-6.24	111.86	120.71
1	A	33	GLY	C-N-CA	-6.24	111.86	120.71
1	C	281	ALA	CA-C-N	6.24	125.92	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	ALA	C-N-CA	6.24	125.92	119.56
2	D	273	ALA	O-C-N	-6.24	115.36	122.09
1	C	306	MET	CA-C-O	-6.23	114.27	120.82
2	D	461	THR	O-C-N	-6.23	114.53	123.07
2	B	298	ARG	CB-CG-CD	6.23	125.64	111.30
1	C	359	HIS	CE1-NE2-CD2	-6.23	102.77	109.00
2	D	404	TYR	CA-CB-CG	6.23	125.11	113.90
1	C	180	VAL	CA-C-N	6.23	128.95	120.54
1	C	180	VAL	C-N-CA	6.23	128.95	120.54
2	B	268	GLU	CA-C-O	-6.23	114.22	121.07
2	B	422	GLU	CA-CB-CG	6.22	126.55	114.10
1	C	38	TRP	N-CA-C	-6.22	100.69	109.96
2	D	364	THR	CA-C-N	6.22	130.65	120.63
2	D	364	THR	C-N-CA	6.22	130.65	120.63
1	A	130	PRO	N-CA-CB	6.22	110.11	103.39
1	C	156	ILE	CA-CB-CG1	6.22	120.98	110.40
2	D	217	LEU	CA-CB-CG	6.22	138.07	116.30
1	C	324	SER	CA-C-N	-6.22	114.76	122.84
1	C	324	SER	C-N-CA	-6.22	114.76	122.84
2	D	455	ASN	OD1-CG-ND2	-6.22	116.38	122.60
2	D	117	ASP	CA-C-O	6.21	127.51	120.80
2	D	455	ASN	CA-C-N	6.21	131.69	122.74
2	D	455	ASN	C-N-CA	6.21	131.69	122.74
1	C	491	GLU	N-CA-C	6.21	118.85	111.33
1	C	510	ALA	CA-C-N	6.21	129.43	120.79
1	C	510	ALA	C-N-CA	6.21	129.43	120.79
2	D	187	ASP	N-CA-C	6.21	119.89	112.93
1	C	315	PHE	CA-CB-CG	-6.21	107.59	113.80
1	C	438	GLU	O-C-N	-6.21	115.54	122.12
1	A	639	GLU	N-CA-CB	-6.21	100.66	110.22
1	A	666	PRO	N-CA-CB	6.21	110.16	103.33
2	B	632	ASP	O-C-N	-6.21	114.33	122.59
1	C	235	TRP	N-CA-C	6.21	119.63	109.76
2	B	504	SER	CA-C-O	6.21	127.11	120.10
1	C	601	LEU	N-CA-CB	6.21	120.53	110.42
1	C	169	GLY	CA-C-O	6.20	131.36	120.57
1	A	92	PHE	CA-C-O	-6.20	114.07	120.89
1	C	722	LEU	CA-C-O	-6.20	114.49	121.00
1	C	195	THR	CA-CB-CG2	6.20	121.03	110.50
1	C	613	GLY	O-C-N	-6.20	116.18	122.19
1	A	392	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	C	369	ASP	CA-C-O	6.19	126.92	119.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LEU	N-CA-C	6.19	120.30	112.87
1	C	528	ASP	N-CA-C	6.19	120.44	113.01
2	B	596	SER	CA-C-O	-6.19	114.42	121.66
2	D	147	PRO	O-C-N	-6.19	115.12	122.24
2	D	204	PHE	CA-C-N	6.19	128.82	120.65
2	D	204	PHE	C-N-CA	6.19	128.82	120.65
2	B	296	ARG	CD-NE-CZ	6.18	133.06	124.40
2	B	528	GLU	CA-C-N	6.18	133.53	121.41
2	B	528	GLU	C-N-CA	6.18	133.53	121.41
1	C	107	ALA	O-C-N	-6.18	114.35	122.39
1	C	602	LEU	CA-C-N	-6.18	112.98	122.62
1	C	602	LEU	C-N-CA	-6.18	112.98	122.62
2	B	336	PRO	N-CA-CB	6.18	110.06	103.39
1	C	168	ASN	CB-CG-ND2	-6.18	107.14	116.40
1	C	169	GLY	O-C-N	-6.18	114.67	122.70
1	C	586	LEU	CA-C-N	6.18	128.47	120.56
1	C	586	LEU	C-N-CA	6.18	128.47	120.56
1	A	485	ASN	CB-CG-ND2	-6.17	107.14	116.40
1	C	636	THR	CB-CA-C	-6.17	100.70	109.96
1	A	308	TRP	O-C-N	-6.17	115.71	122.07
1	A	517	TRP	CA-C-O	6.17	127.86	121.07
2	B	586	LYS	CA-C-N	6.17	129.17	120.28
2	B	586	LYS	C-N-CA	6.17	129.17	120.28
2	B	35	TRP	CB-CA-C	6.17	120.57	110.88
1	A	452	ARG	N-CA-CB	6.17	118.95	110.01
1	C	40	THR	O-C-N	-6.17	115.82	122.85
1	C	180	VAL	O-C-N	-6.17	115.87	121.91
1	C	684	VAL	O-C-N	-6.17	116.50	123.10
1	C	80	ALA	N-CA-C	-6.16	103.87	111.33
2	D	447	ALA	N-CA-C	-6.16	104.19	111.03
2	D	200	ASP	CA-C-N	6.16	125.38	118.97
2	D	200	ASP	C-N-CA	6.16	125.38	118.97
1	C	477	PRO	N-CA-CB	6.16	108.73	103.19
1	A	186	GLY	CA-C-N	-6.16	115.02	122.90
1	A	186	GLY	C-N-CA	-6.16	115.02	122.90
1	C	627	ASP	CA-C-N	-6.16	115.07	123.14
1	C	627	ASP	C-N-CA	-6.16	115.07	123.14
1	C	231	ASN	N-CA-C	6.16	122.25	114.31
2	D	49	PRO	N-CA-CB	6.16	110.19	103.30
2	D	260	ALA	CA-C-O	-6.15	114.31	120.90
1	A	10	VAL	N-CA-CB	-6.15	103.99	110.82
1	A	157	PRO	N-CA-CB	6.15	109.71	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	SER	CA-C-N	6.15	128.44	120.44
1	A	549	SER	C-N-CA	6.15	128.44	120.44
2	B	378	ILE	CA-C-O	6.15	127.69	121.17
2	D	634	LEU	CA-C-N	6.15	133.47	121.41
2	D	634	LEU	C-N-CA	6.15	133.47	121.41
1	A	155	GLY	CA-C-N	6.15	133.51	122.13
1	A	155	GLY	C-N-CA	6.15	133.51	122.13
1	A	586	LEU	N-CA-C	6.15	119.62	111.75
2	B	629	SER	CA-C-N	6.15	128.52	120.28
2	B	629	SER	C-N-CA	6.15	128.52	120.28
1	C	700	GLY	CA-C-O	-6.15	114.60	119.83
1	A	118	ASP	N-CA-CB	6.15	119.15	110.36
2	B	403	TYR	CA-C-O	6.14	127.27	120.82
1	A	196	ILE	N-CA-C	-6.14	99.28	108.12
2	D	75	MET	N-CA-CB	-6.14	100.50	110.81
2	D	142	PRO	CA-C-O	6.14	128.88	119.55
2	D	421	GLN	O-C-N	-6.14	114.77	122.20
1	A	475	GLU	CA-CB-CG	6.14	126.37	114.10
2	B	562	ALA	O-C-N	6.13	130.10	122.86
1	A	10	VAL	N-CA-C	6.13	116.94	108.84
1	A	361	GLN	N-CA-C	-6.13	104.87	112.90
1	A	526	ASP	CA-C-N	6.13	126.03	119.28
1	A	526	ASP	C-N-CA	6.13	126.03	119.28
2	B	630	THR	O-C-N	-6.13	115.62	122.12
1	C	628	VAL	CA-C-O	-6.13	113.95	120.39
1	C	189	PRO	N-CA-CB	6.13	110.01	103.39
2	B	87	TYR	CA-C-N	6.13	126.31	120.31
2	B	87	TYR	C-N-CA	6.13	126.31	120.31
1	C	98	SER	O-C-N	-6.12	115.72	122.09
2	B	86	GLY	CA-C-N	6.12	137.68	122.74
2	B	86	GLY	C-N-CA	6.12	137.68	122.74
1	A	359	HIS	CA-C-O	6.12	129.26	120.51
2	D	79	LYS	CA-C-O	-6.12	114.07	120.92
2	B	104	MET	CA-C-O	-6.11	114.07	120.55
2	B	268	GLU	CB-CA-C	-6.11	101.20	110.92
1	C	78	MET	CA-C-O	6.11	128.93	119.21
1	C	616	VAL	CA-C-O	-6.11	114.27	121.05
1	C	185	GLN	N-CA-CB	6.11	120.05	110.46
2	B	139	ARG	CA-C-N	-6.11	114.81	123.11
2	B	139	ARG	C-N-CA	-6.11	114.81	123.11
1	C	188	LYS	CA-C-N	6.11	126.00	119.28
1	C	188	LYS	C-N-CA	6.11	126.00	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	288	HIS	CB-CG-ND1	-6.10	113.55	122.70
1	A	140	GLY	O-C-N	-6.10	117.71	123.81
2	B	128	GLY	O-C-N	-6.10	116.27	122.19
1	A	161	MET	CA-CB-CG	6.10	126.30	114.10
1	A	401	ASP	CA-C-O	6.10	128.51	120.16
1	C	475	GLU	N-CA-CB	6.09	118.22	110.23
2	D	113	HIS	CA-CB-CG	-6.09	107.71	113.80
1	A	195	THR	CA-CB-CG2	6.09	120.86	110.50
1	A	40	THR	O-C-N	-6.09	115.16	122.65
1	A	408	TYR	N-CA-C	-6.09	104.27	111.03
2	B	240	ILE	CA-C-O	-6.09	114.72	121.17
2	B	259	GLY	CA-C-O	-6.08	114.43	121.00
1	C	147	TYR	CA-C-N	6.08	128.35	120.44
1	C	147	TYR	C-N-CA	6.08	128.35	120.44
2	D	133	VAL	CA-C-O	-6.08	113.59	120.95
2	B	154	LEU	CA-C-O	6.08	126.89	119.11
2	D	308	GLY	CA-C-N	6.08	130.98	120.58
2	D	308	GLY	C-N-CA	6.08	130.98	120.58
2	D	463	VAL	CA-C-O	-6.08	113.18	120.78
2	D	165	GLU	N-CA-CB	6.08	121.41	110.83
1	C	512	LEU	O-C-N	-6.08	115.71	122.03
1	C	573	GLU	CA-C-O	-6.08	111.82	120.51
1	C	714	SER	O-C-N	-6.08	115.68	122.12
2	B	268	GLU	CA-CB-CG	6.08	126.25	114.10
1	C	344	ASN	CA-CB-CG	6.08	118.68	112.60
2	D	39	VAL	CA-C-O	-6.08	114.73	121.17
2	D	571	ALA	CA-C-N	6.08	128.34	120.44
2	D	571	ALA	C-N-CA	6.08	128.34	120.44
1	A	221	ILE	CA-CB-CG1	6.07	120.72	110.40
1	A	262	ASP	N-CA-C	-6.07	104.57	111.07
2	D	331	LEU	N-CA-CB	6.07	118.97	110.04
2	B	24	ALA	O-C-N	-6.07	115.23	122.15
1	A	586	LEU	O-C-N	-6.07	115.28	122.20
1	C	475	GLU	CA-CB-CG	6.07	126.23	114.10
2	B	394	ARG	O-C-N	-6.06	113.42	122.39
2	D	337	TYR	CA-C-O	-6.06	113.25	120.10
2	D	56	ALA	CA-C-O	-6.06	114.46	120.82
1	A	588	GLU	N-CA-C	-6.06	104.59	111.07
1	A	704	ILE	O-C-N	-6.06	116.88	123.18
1	C	208	ASN	CB-CG-ND2	6.06	125.49	116.40
2	D	173	GLY	N-CA-C	-6.06	105.47	112.50
1	A	684	VAL	N-CA-CB	6.06	119.77	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	32	GLU	CA-C-O	6.06	126.97	120.55
2	D	265	ALA	CA-C-N	6.06	132.67	121.52
2	D	265	ALA	C-N-CA	6.06	132.67	121.52
1	C	357	GLN	OE1-CD-NE2	6.05	128.66	122.60
1	C	456	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	A	191	GLN	OE1-CD-NE2	-6.05	116.55	122.60
2	B	598	ALA	O-C-N	-6.05	115.53	123.16
2	D	548	GLY	N-CA-C	6.05	121.83	112.45
1	C	278	ASP	O-C-N	-6.05	114.11	122.46
2	D	487	GLY	O-C-N	6.05	128.43	122.92
1	A	261	ALA	CB-CA-C	6.05	122.29	110.67
1	C	174	ILE	N-CA-CB	-6.05	101.51	110.58
1	C	173	PRO	N-CA-CB	6.05	109.98	103.33
1	A	175	LEU	O-C-N	-6.05	115.84	122.07
2	D	271	PHE	CA-C-O	-6.05	114.21	121.89
1	A	102	TYR	CA-CB-CG	6.04	124.78	113.90
1	C	646	GLU	CA-CB-CG	6.04	126.18	114.10
1	C	91	GLY	O-C-N	-6.04	114.85	122.70
1	A	123	ARG	N-CA-C	6.04	119.69	112.93
2	B	159	LEU	O-C-N	-6.04	114.56	122.59
2	B	278	ASP	CA-C-O	-6.04	111.88	120.51
1	A	590	PHE	CB-CA-C	-6.03	101.41	110.88
1	A	298	VAL	O-C-N	-6.03	116.00	121.91
2	B	437	HIS	CA-CB-CG	-6.03	107.77	113.80
1	A	543	ALA	O-C-N	-6.03	115.92	122.79
1	C	218	MET	CB-CA-C	6.03	120.80	110.79
1	C	442	PRO	N-CA-CB	6.03	109.58	103.25
1	C	245	MET	N-CA-C	-6.03	104.63	111.14
1	A	622	ALA	N-CA-C	-6.03	104.62	111.07
2	D	627	LEU	CB-CA-C	6.03	120.24	110.96
1	C	94	THR	CA-C-N	6.02	128.67	120.54
1	C	94	THR	C-N-CA	6.02	128.67	120.54
1	C	697	ARG	O-C-N	-6.02	115.83	122.09
2	D	208	GLN	CA-C-O	6.02	126.65	119.60
1	A	225	PHE	CA-CB-CG	6.02	119.82	113.80
2	D	456	ARG	O-C-N	-6.02	112.14	122.20
2	B	163	LYS	CA-C-O	-6.02	114.42	121.16
1	A	350	ILE	O-C-N	-6.02	116.03	121.87
2	D	72	ILE	O-C-N	6.02	129.58	123.20
1	A	295	PHE	N-CA-C	6.02	118.80	111.82
2	D	172	GLN	CA-C-O	6.02	126.93	120.55
2	D	580	GLU	CA-CB-CG	6.02	126.13	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	THR	N-CA-CB	6.01	118.73	110.01
1	C	278	ASP	N-CA-CB	6.01	120.92	110.39
1	C	476	PRO	CA-C-N	6.01	126.36	119.93
1	C	476	PRO	C-N-CA	6.01	126.36	119.93
1	C	148	ASP	N-CA-CB	-6.01	101.30	110.01
1	A	330	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	C	247	GLU	O-C-N	-6.01	115.19	122.22
1	A	570	TYR	CA-C-N	6.00	128.25	120.44
1	A	570	TYR	C-N-CA	6.00	128.25	120.44
2	B	311	PHE	O-C-N	-6.00	113.50	122.39
2	D	185	ARG	O-C-N	-6.00	114.61	122.59
1	A	352	ALA	CA-C-O	6.00	126.91	120.55
1	C	688	ILE	CA-C-N	5.99	125.93	119.76
1	C	688	ILE	C-N-CA	5.99	125.93	119.76
2	D	490	TRP	CA-C-N	5.99	132.40	122.33
2	D	490	TRP	C-N-CA	5.99	132.40	122.33
2	D	574	TYR	N-CA-C	5.99	118.58	111.33
1	C	187	VAL	N-CA-CB	-5.99	103.91	111.46
2	D	92	PRO	N-CA-C	5.99	127.68	112.10
2	B	517	CYS	CA-C-N	-5.99	113.96	122.94
2	B	517	CYS	C-N-CA	-5.99	113.96	122.94
1	A	40	THR	CA-CB-CG2	5.99	120.67	110.50
2	B	425	LYS	CA-CB-CG	5.99	126.07	114.10
1	C	502	GLU	N-CA-C	5.99	119.68	112.38
1	C	642	ARG	CA-C-N	5.98	128.22	120.44
1	C	642	ARG	C-N-CA	5.98	128.22	120.44
2	D	104	MET	CB-CA-C	5.98	120.77	110.84
2	B	290	GLN	CB-CG-CD	5.98	122.77	112.60
2	B	480	PRO	N-CA-CB	5.98	108.52	103.25
1	A	208	ASN	N-CA-C	5.98	119.89	112.24
2	D	35	TRP	N-CA-C	-5.98	104.45	110.97
1	A	498	LYS	CA-C-N	5.98	128.61	120.54
1	A	498	LYS	C-N-CA	5.98	128.61	120.54
1	A	262	ASP	N-CA-CB	5.97	118.67	110.01
2	B	299	ALA	CA-C-N	5.97	128.21	120.44
2	B	299	ALA	C-N-CA	5.97	128.21	120.44
1	A	320	PRO	O-C-N	-5.97	115.06	122.23
1	A	703	GLU	CA-C-N	5.97	131.46	122.98
1	A	703	GLU	C-N-CA	5.97	131.46	122.98
1	C	552	LEU	CA-C-N	5.97	128.88	120.28
1	C	552	LEU	C-N-CA	5.97	128.88	120.28
2	D	380	ARG	N-CA-CB	5.97	118.66	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	262	TYR	N-CA-C	5.96	118.57	111.71
2	B	274	THR	CA-C-O	-5.96	114.23	120.55
2	B	510	ARG	CA-C-N	5.96	125.92	119.78
2	B	510	ARG	C-N-CA	5.96	125.92	119.78
2	D	472	ARG	CB-CG-CD	5.96	125.01	111.30
1	A	103	ARG	CA-C-O	5.96	126.74	120.42
2	B	55	PHE	N-CA-CB	5.96	118.65	110.01
2	B	113	HIS	CA-C-O	5.96	126.56	120.24
1	C	126	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	690	GLU	O-C-N	-5.96	115.40	122.20
1	A	505	PRO	CA-C-O	-5.96	110.66	119.18
2	B	315	GLU	N-CA-C	5.96	120.09	112.34
2	B	374	PHE	CA-C-N	5.96	125.66	119.05
2	B	374	PHE	C-N-CA	5.96	125.66	119.05
2	B	376	LEU	CA-C-N	5.96	128.26	120.28
2	B	376	LEU	C-N-CA	5.96	128.26	120.28
1	C	100	ALA	O-C-N	-5.96	115.93	122.07
1	C	399	VAL	N-CA-C	5.96	116.51	108.17
2	D	182	VAL	CA-C-O	-5.96	115.07	121.27
1	A	445	ARG	O-C-N	-5.95	115.81	122.12
2	B	230	ASP	N-CA-C	-5.95	104.73	112.23
1	C	120	PRO	CA-C-N	5.95	128.58	120.54
1	C	120	PRO	C-N-CA	5.95	128.58	120.54
2	B	72	ILE	O-C-N	5.95	129.51	123.20
1	A	52	GLU	CA-CB-CG	5.95	126.00	114.10
1	A	411	GLU	CA-C-O	-5.95	114.57	120.82
2	D	297	LEU	CA-C-N	5.95	130.80	120.68
2	D	297	LEU	C-N-CA	5.95	130.80	120.68
2	B	405	VAL	CA-C-O	-5.95	114.76	120.95
1	C	652	VAL	N-CA-CB	5.95	118.84	111.41
2	B	551	ALA	CA-C-O	-5.95	114.06	121.02
1	C	269	ALA	CA-C-N	5.95	126.58	119.98
1	C	269	ALA	C-N-CA	5.95	126.58	119.98
1	A	393	GLU	N-CA-C	5.94	120.81	113.50
2	B	222	ARG	CA-C-N	5.94	128.24	120.28
2	B	222	ARG	C-N-CA	5.94	128.24	120.28
1	C	438	GLU	CB-CA-C	5.94	120.65	110.79
1	C	570	TYR	N-CA-C	5.94	118.24	111.11
1	A	666	PRO	CA-C-O	5.94	129.13	119.86
1	C	206	VAL	CB-CA-C	-5.94	101.55	111.29
2	D	133	VAL	N-CA-C	-5.94	101.00	108.84
2	D	636	VAL	N-CA-C	-5.94	99.86	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	B	388	GLU	N-CA-C	5.93	120.67	112.90
1	C	510	ALA	N-CA-C	-5.93	104.50	110.97
2	D	152	GLU	CA-CB-CG	-5.93	102.23	114.10
2	B	170	TYR	N-CA-C	5.93	121.56	113.97
1	C	219	ARG	NE-CZ-NH2	-5.93	113.86	119.20
2	D	543	PRO	N-CA-CB	5.93	108.51	103.35
2	D	235	THR	CA-CB-CG2	5.93	120.58	110.50
1	A	101	PHE	CA-C-O	-5.93	114.60	120.82
2	B	505	THR	CA-C-N	5.92	128.54	120.54
2	B	505	THR	C-N-CA	5.92	128.54	120.54
1	C	407	ALA	N-CA-C	5.92	117.82	111.36
1	C	526	ASP	CA-CB-CG	5.92	118.52	112.60
2	B	20	THR	O-C-N	-5.92	113.52	123.00
2	B	105	ASP	O-C-N	-5.92	115.31	122.71
2	B	322	GLN	CA-C-O	5.92	126.75	120.36
2	B	461	THR	N-CA-CB	5.92	118.86	109.51
1	C	74	PRO	N-CA-CB	5.92	110.07	103.44
1	A	150	ARG	NH1-CZ-NH2	5.92	126.99	119.30
1	A	727	ASP	N-CA-CB	5.92	119.40	110.11
1	C	136	VAL	N-CA-CB	5.92	117.30	110.49
1	C	332	SER	CA-C-N	5.92	126.51	120.00
1	C	332	SER	C-N-CA	5.92	126.51	120.00
1	A	679	ASP	N-CA-CB	5.92	119.02	110.20
2	B	302	GLU	N-CA-C	5.92	117.73	111.28
1	C	626	PHE	CA-C-N	-5.92	114.56	122.72
1	C	626	PHE	C-N-CA	-5.92	114.56	122.72
2	B	629	SER	O-C-N	-5.92	115.75	122.08
2	D	521	ARG	CB-CA-C	5.91	121.57	110.63
2	B	543	PRO	N-CA-CB	5.91	108.57	103.31
2	B	564	VAL	CA-CB-CG2	5.91	120.45	110.40
1	C	676	GLY	CA-C-N	5.91	127.48	122.28
1	C	676	GLY	C-N-CA	5.91	127.48	122.28
1	C	406	SER	CA-C-N	-5.91	111.90	120.29
1	C	406	SER	C-N-CA	-5.91	111.90	120.29
1	C	504	ASP	CA-C-N	5.91	125.45	119.19
1	C	504	ASP	C-N-CA	5.91	125.45	119.19
1	A	225	PHE	CA-C-N	5.91	128.51	120.54
1	A	225	PHE	C-N-CA	5.91	128.51	120.54
1	A	675	LEU	O-C-N	-5.91	112.91	122.42
1	A	582	GLU	O-C-N	-5.90	115.86	122.12
1	C	493	LYS	O-C-N	-5.90	115.95	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	VAL	N-CA-CB	5.90	117.85	110.47
2	D	89	GLY	N-CA-C	5.90	127.17	113.18
2	D	390	VAL	CA-C-O	5.90	126.03	119.42
2	D	475	GLU	N-CA-CB	5.90	118.66	110.17
2	D	54	THR	CB-CA-C	-5.90	100.25	110.45
2	D	388	GLU	N-CA-C	5.90	118.94	111.69
1	A	363	LEU	N-CA-CB	-5.90	100.55	111.52
2	B	496	VAL	CA-C-N	5.89	129.27	120.31
2	B	496	VAL	C-N-CA	5.89	129.27	120.31
2	B	322	GLN	OE1-CD-NE2	-5.89	116.71	122.60
2	D	363	PHE	N-CA-C	5.89	118.49	111.71
1	A	150	ARG	CA-C-N	5.89	130.65	120.58
1	A	150	ARG	C-N-CA	5.89	130.65	120.58
1	A	521	ASN	CA-C-O	5.89	128.57	120.80
1	C	475	GLU	CA-C-O	5.89	123.68	119.32
1	A	639	GLU	O-C-N	-5.89	115.33	122.22
2	B	451	LYS	O-C-N	-5.89	115.73	122.09
2	B	582	ALA	CA-C-O	-5.89	114.82	121.00
1	A	104	ARG	CA-C-N	5.88	128.17	120.28
1	A	104	ARG	C-N-CA	5.88	128.17	120.28
1	A	197	GLN	CA-CB-CG	-5.88	102.33	114.10
1	A	608	ASP	CA-C-O	5.88	127.16	120.80
2	B	84	LYS	CA-C-O	5.88	126.76	120.46
2	B	210	THR	N-CA-CB	5.88	120.26	110.14
2	D	583	LYS	CA-C-N	5.88	128.48	120.54
2	D	583	LYS	C-N-CA	5.88	128.48	120.54
2	D	421	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	328	HIS	N-CA-C	-5.88	101.30	110.42
2	B	416	ALA	O-C-N	-5.88	114.45	122.33
1	C	174	ILE	N-CA-C	5.88	116.66	110.72
2	D	502	ASP	N-CA-CB	5.88	118.86	110.16
2	B	350	ALA	CA-C-N	5.88	128.15	120.28
2	B	350	ALA	C-N-CA	5.88	128.15	120.28
2	B	604	ASP	CA-C-N	5.88	132.24	122.54
2	B	604	ASP	C-N-CA	5.88	132.24	122.54
1	C	375	PRO	CB-CA-C	-5.88	104.10	111.56
1	A	391	GLN	CA-C-N	5.88	130.40	120.88
1	A	391	GLN	C-N-CA	5.88	130.40	120.88
2	D	500	LEU	CA-C-N	5.87	128.08	120.44
2	D	500	LEU	C-N-CA	5.87	128.08	120.44
1	C	95	ALA	CA-C-N	5.87	128.07	120.44
1	C	95	ALA	C-N-CA	5.87	128.07	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ILE	O-C-N	-5.87	115.23	122.57
2	D	160	GLU	CA-C-N	5.87	130.51	120.71
2	D	160	GLU	C-N-CA	5.87	130.51	120.71
1	A	76	ALA	N-CA-C	5.87	118.46	111.71
1	C	304	ALA	CA-C-N	5.87	128.07	120.44
1	C	304	ALA	C-N-CA	5.87	128.07	120.44
1	C	606	GLY	O-C-N	-5.87	117.33	122.90
2	D	38	GLU	CA-C-O	-5.87	114.66	120.82
1	A	587	VAL	CB-CA-C	5.87	120.10	112.24
2	B	407	SER	CA-C-N	5.87	128.73	120.28
2	B	407	SER	C-N-CA	5.87	128.73	120.28
1	A	55	TYR	N-CA-C	5.86	118.62	111.82
2	B	108	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	342	TYR	CA-C-N	5.86	128.72	120.28
1	C	342	TYR	C-N-CA	5.86	128.72	120.28
1	A	209	THR	CA-CB-CG2	5.86	120.47	110.50
1	A	96	LYS	CA-CB-CG	-5.86	102.38	114.10
2	B	442	LEU	N-CA-C	-5.86	104.80	111.07
2	B	481	ALA	N-CA-C	5.86	118.32	110.35
1	C	640	THR	CB-CA-C	5.86	120.16	110.90
2	B	115	ASP	CB-CG-OD1	5.86	131.87	118.40
1	C	189	PRO	O-C-N	-5.86	114.67	122.22
2	B	466	PHE	CA-C-O	5.86	124.94	120.26
1	C	351	GLU	CA-C-N	5.86	128.05	120.44
1	C	351	GLU	C-N-CA	5.86	128.05	120.44
2	D	74	PRO	CA-C-O	5.86	127.95	119.34
1	C	524	ASP	O-C-N	-5.85	114.38	122.46
2	B	377	ARG	O-C-N	-5.85	115.92	122.12
1	A	392	GLN	O-C-N	5.85	128.90	122.11
1	A	516	THR	N-CA-C	5.85	117.65	111.28
2	B	396	ASN	N-CA-CB	5.85	119.01	109.95
1	C	198	ASN	N-CA-CB	-5.85	103.13	111.84
2	B	66	THR	CA-C-N	5.85	130.21	120.62
2	B	66	THR	C-N-CA	5.85	130.21	120.62
1	C	679	ASP	N-CA-C	-5.85	105.24	112.90
1	A	207	ARG	CA-C-O	5.84	126.10	119.27
2	B	224	LEU	CA-C-N	5.84	130.03	120.63
2	B	224	LEU	C-N-CA	5.84	130.03	120.63
2	B	426	LEU	CB-CA-C	-5.84	99.02	110.11
1	C	23	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	679	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	697	ARG	CA-C-N	5.84	128.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	ARG	C-N-CA	5.84	128.68	120.28
2	D	124	ALA	O-C-N	-5.84	116.02	122.09
2	D	510	ARG	CD-NE-CZ	5.84	132.57	124.40
1	C	276	ASN	O-C-N	-5.83	115.97	122.86
1	A	665	VAL	N-CA-C	5.83	119.35	112.35
2	B	49	PRO	N-CA-C	5.83	124.49	112.47
2	D	80	ASP	CA-C-O	-5.83	112.17	120.51
2	D	353	GLY	CA-C-O	-5.83	114.70	121.00
1	C	30	ALA	CB-CA-C	5.83	120.14	110.81
1	A	645	VAL	CB-CA-C	5.83	119.39	111.87
1	C	520	GLY	CA-C-O	5.83	126.70	120.40
1	A	674	LYS	N-CA-C	-5.83	105.06	111.82
2	D	74	PRO	CA-C-N	5.83	132.12	122.33
2	D	74	PRO	C-N-CA	5.83	132.12	122.33
2	D	114	GLU	CA-CB-CG	5.83	125.76	114.10
1	A	510	ALA	CA-C-N	5.83	128.40	120.54
1	A	510	ALA	C-N-CA	5.83	128.40	120.54
1	C	52	GLU	N-CA-C	5.83	123.21	110.80
2	D	340	ILE	O-C-N	-5.83	116.22	121.87
2	D	223	ARG	O-C-N	-5.82	115.95	122.12
1	A	298	VAL	N-CA-C	-5.82	104.83	110.42
1	C	190	GLU	CB-CG-CD	5.82	122.50	112.60
1	C	434	ALA	CA-C-N	5.82	128.00	120.44
1	C	434	ALA	C-N-CA	5.82	128.00	120.44
1	A	31	LYS	O-C-N	-5.82	115.41	122.22
2	B	55	PHE	O-C-N	-5.82	116.08	122.07
2	B	107	TRP	CA-C-O	5.82	129.28	121.89
2	B	450	ALA	O-C-N	-5.82	115.57	122.20
2	D	329	ARG	CA-CB-CG	-5.82	102.46	114.10
1	A	635	GLN	CA-C-O	-5.82	114.65	121.16
2	B	458	GLN	CG-CD-NE2	5.81	125.12	116.40
1	C	591	GLU	O-C-N	-5.81	115.96	122.12
2	D	494	SER	CA-C-N	5.81	127.99	120.44
2	D	494	SER	C-N-CA	5.81	127.99	120.44
1	C	31	LYS	CA-C-N	5.81	128.54	120.29
1	C	31	LYS	C-N-CA	5.81	128.54	120.29
1	C	432	GLY	N-CA-C	5.81	117.95	112.08
2	B	261	GLU	CB-CA-C	-5.81	101.76	110.88
1	C	20	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	345	VAL	CA-C-N	5.81	127.88	120.56
1	C	345	VAL	C-N-CA	5.81	127.88	120.56
1	A	698	LYS	O-C-N	-5.81	115.43	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ALA	O-C-N	-5.80	116.09	122.07
2	B	109	VAL	N-CA-C	-5.80	99.35	108.23
1	C	469	LYS	CB-CG-CD	-5.80	97.95	111.30
1	C	593	ALA	O-C-N	-5.80	115.76	122.03
1	C	675	LEU	CA-C-N	5.80	132.79	121.41
1	C	675	LEU	C-N-CA	5.80	132.79	121.41
2	D	220	TRP	N-CA-C	-5.80	104.87	111.14
2	B	477	LYS	CA-CB-CG	5.80	125.71	114.10
1	C	43	GLN	O-C-N	-5.80	115.62	122.58
2	D	149	HIS	N-CA-C	-5.80	105.86	113.17
1	A	519	ALA	O-C-N	-5.80	116.10	122.07
2	B	100	ARG	NE-CZ-NH2	-5.80	113.98	119.20
2	B	464	SER	N-CA-C	-5.80	106.55	113.97
2	D	232	ARG	NH1-CZ-NH2	-5.80	111.76	119.30
1	A	517	TRP	CA-C-N	5.80	128.05	120.28
1	A	517	TRP	C-N-CA	5.80	128.05	120.28
2	B	382	THR	CA-C-N	5.79	126.37	119.94
2	B	382	THR	C-N-CA	5.79	126.37	119.94
1	C	210	TYR	O-C-N	-5.79	116.18	122.79
2	D	170	TYR	N-CA-CB	5.79	118.87	110.88
2	B	445	CYS	CA-C-O	5.79	126.90	120.82
2	B	622	ASP	CB-CA-C	5.79	119.89	110.22
1	A	18	PRO	N-CA-CB	5.79	108.39	103.35
1	A	18	PRO	O-C-N	-5.79	115.83	123.01
1	C	488	VAL	CA-C-N	5.79	128.84	120.79
1	C	488	VAL	C-N-CA	5.79	128.84	120.79
2	D	574	TYR	O-C-N	-5.79	115.98	122.12
1	A	95	ALA	CA-C-N	5.79	127.96	120.44
1	A	95	ALA	C-N-CA	5.79	127.96	120.44
2	D	311	PHE	O-C-N	-5.79	114.93	122.39
2	D	380	ARG	NH1-CZ-NH2	-5.78	111.78	119.30
1	A	229	SER	N-CA-C	5.78	117.58	111.28
1	A	512	LEU	O-C-N	-5.78	116.02	122.03
1	A	449	ALA	CA-C-N	5.78	128.50	120.29
1	A	449	ALA	C-N-CA	5.78	128.50	120.29
1	A	213	PRO	CA-C-N	5.78	127.06	119.84
1	A	213	PRO	C-N-CA	5.78	127.06	119.84
1	A	412	LEU	N-CA-C	-5.78	104.89	111.07
2	B	223	ARG	NH1-CZ-NH2	5.78	126.81	119.30
2	D	247	GLY	N-CA-C	-5.78	99.49	113.18
1	A	385	ASN	CA-C-N	5.77	128.33	120.54
1	A	385	ASN	C-N-CA	5.77	128.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	274	THR	CA-C-N	5.77	131.25	121.14
2	D	274	THR	C-N-CA	5.77	131.25	121.14
1	A	23	ARG	O-C-N	-5.77	115.47	122.22
2	D	57	GLU	N-CA-C	-5.77	104.91	111.14
2	B	492	ARG	CA-C-O	-5.77	115.43	121.55
1	C	546	GLY	N-CA-C	-5.77	105.51	112.49
2	D	351	SER	N-CA-CB	5.77	118.54	109.94
1	A	369	ASP	CA-CB-CG	5.77	118.37	112.60
2	B	293	THR	N-CA-C	-5.77	104.90	111.07
2	D	39	VAL	O-C-N	-5.77	116.26	121.91
1	C	577	THR	CA-CB-CG2	5.77	120.30	110.50
1	A	23	ARG	NE-CZ-NH1	5.76	127.27	121.50
2	B	340	ILE	O-C-N	-5.76	115.89	121.83
1	C	61	LEU	CA-C-N	5.76	132.55	121.54
1	C	61	LEU	C-N-CA	5.76	132.55	121.54
1	C	94	THR	O-C-N	-5.76	116.52	123.03
1	C	121	THR	O-C-N	-5.76	116.10	122.09
1	A	346	VAL	CA-C-O	-5.76	115.07	121.17
1	A	406	SER	O-C-N	-5.76	116.15	123.06
1	A	637	PRO	N-CA-CB	5.76	109.66	103.33
1	A	707	PRO	N-CA-CB	5.76	108.32	103.25
1	C	595	GLY	CA-C-O	5.76	126.21	119.19
2	D	522	ARG	CD-NE-CZ	5.76	132.46	124.40
1	A	445	ARG	CA-C-O	5.75	126.65	120.55
2	D	214	LEU	N-CA-CB	-5.75	102.13	110.47
1	A	49	LEU	O-C-N	-5.75	116.68	123.41
2	D	183	TYR	CA-C-N	5.75	130.34	121.19
2	D	183	TYR	C-N-CA	5.75	130.34	121.19
1	A	512	LEU	CA-C-N	5.75	129.44	120.82
1	A	512	LEU	C-N-CA	5.75	129.44	120.82
2	B	241	TYR	CA-C-N	5.75	128.45	120.29
2	B	241	TYR	C-N-CA	5.75	128.45	120.29
2	D	304	TRP	O-C-N	-5.75	116.11	122.09
1	A	59	ASP	CA-C-O	-5.75	112.33	119.28
1	A	305	ARG	O-C-N	-5.75	116.03	122.12
1	A	357	GLN	CA-C-O	5.75	126.46	119.11
1	C	693	PHE	CA-CB-CG	5.75	119.55	113.80
2	D	552	GLU	N-CA-C	5.75	118.32	111.71
2	D	220	TRP	CA-C-O	-5.74	114.78	120.70
1	A	270	GLY	CA-C-N	5.74	127.97	120.28
1	A	270	GLY	C-N-CA	5.74	127.97	120.28
2	B	297	LEU	CA-C-N	5.74	128.25	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	297	LEU	C-N-CA	5.74	128.25	120.44
2	D	99	VAL	CA-C-O	-5.74	115.09	121.23
2	D	443	ASP	CA-C-O	-5.74	113.62	120.10
2	D	189	PRO	N-CA-CB	5.74	109.27	103.25
1	C	394	SER	CA-CB-OG	5.73	122.57	111.10
1	C	2	SER	CA-C-N	5.73	132.48	121.54
1	C	2	SER	C-N-CA	5.73	132.48	121.54
1	C	39	GLU	CB-CG-CD	5.73	122.34	112.60
2	D	87	TYR	CG-CD2-CE2	5.73	129.80	121.20
2	D	59	LEU	CA-C-N	5.73	128.21	120.65
2	D	59	LEU	C-N-CA	5.73	128.21	120.65
1	A	231	ASN	CB-CA-C	-5.73	100.03	109.99
1	A	712	PRO	N-CA-CB	5.72	109.35	103.23
1	A	216	PRO	O-C-N	-5.72	115.37	122.23
2	B	536	HIS	CA-C-O	-5.72	113.64	120.10
1	C	514	LYS	CB-CA-C	5.72	119.86	110.88
2	D	616	ARG	N-CA-CB	-5.72	101.30	111.08
1	C	42	GLU	CB-CA-C	-5.72	98.51	110.17
1	C	418	ARG	NE-CZ-NH2	5.72	124.34	119.20
2	D	268	GLU	O-C-N	-5.72	116.18	122.07
2	D	553	ILE	N-CA-C	-5.72	105.05	110.42
2	B	269	GLN	N-CA-C	5.71	122.97	110.80
2	D	143	ASP	CA-CB-CG	5.71	118.31	112.60
2	D	455	ASN	O-C-N	-5.71	115.48	122.34
1	A	50	PHE	O-C-N	-5.71	116.62	123.31
1	A	520	GLY	CA-C-N	5.71	130.71	123.34
1	A	520	GLY	C-N-CA	5.71	130.71	123.34
2	B	206	ALA	CA-C-O	-5.71	114.79	120.90
1	C	519	ALA	CA-C-N	5.71	127.28	120.14
1	C	519	ALA	C-N-CA	5.71	127.28	120.14
2	D	119	LYS	N-CA-C	-5.71	104.43	111.40
1	A	359	HIS	ND1-CE1-NE2	5.71	114.11	108.40
2	B	35	TRP	O-C-N	-5.71	116.19	122.07
2	B	172	GLN	O-C-N	-5.71	116.19	122.07
2	B	601	GLU	O-C-N	-5.71	116.07	122.12
1	C	268	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	C	468	ASN	CB-CG-ND2	-5.71	107.84	116.40
1	C	148	ASP	CA-C-O	-5.71	114.83	120.82
1	A	382	ILE	O-C-N	-5.70	116.34	121.87
2	B	293	THR	CA-CB-OG1	5.70	118.16	109.60
2	B	192	ASP	CA-CB-CG	-5.70	106.90	112.60
2	D	196	ASN	CA-C-N	-5.70	112.06	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	196	ASN	C-N-CA	-5.70	112.06	121.92
2	D	535	TRP	O-C-N	-5.70	116.20	122.07
2	D	479	PHE	CB-CA-C	-5.70	100.88	109.26
1	C	522	PRO	N-CA-C	5.70	119.40	110.80
1	A	39	GLU	CA-CB-CG	5.69	125.49	114.10
1	A	57	ASP	CA-C-O	-5.69	112.39	119.28
1	C	282	PRO	N-CA-CB	5.69	109.17	103.48
2	B	436	GLU	CA-CB-CG	5.69	125.48	114.10
1	C	334	TRP	CA-C-N	5.69	129.70	120.60
1	C	334	TRP	C-N-CA	5.69	129.70	120.60
2	B	115	ASP	CA-C-N	5.69	125.36	119.05
2	B	115	ASP	C-N-CA	5.69	125.36	119.05
2	D	89	GLY	O-C-N	-5.68	115.31	122.70
1	A	458	ASP	N-CA-C	5.68	118.20	111.33
2	B	429	MET	CA-CB-CG	5.68	125.47	114.10
2	D	507	VAL	CA-C-N	5.68	128.69	120.79
2	D	507	VAL	C-N-CA	5.68	128.69	120.79
2	B	543	PRO	CA-C-O	-5.68	114.86	121.34
1	A	572	LYS	CA-CB-CG	5.68	125.46	114.10
2	B	330	GLU	CB-CA-C	5.67	122.17	110.31
2	D	130	GLU	O-C-N	-5.67	114.83	122.43
2	B	456	ARG	CA-C-N	5.67	131.07	121.14
2	B	456	ARG	C-N-CA	5.67	131.07	121.14
1	C	411	GLU	N-CA-CB	5.67	118.19	109.91
2	D	83	LYS	N-CA-CB	5.67	119.03	110.30
2	B	493	ASP	N-CA-C	5.67	117.46	111.28
1	A	676	GLY	O-C-N	-5.67	116.29	122.41
1	C	223	GLU	CB-CG-CD	5.67	122.24	112.60
2	D	492	ARG	CA-C-O	-5.67	114.95	121.47
1	A	319	ASN	N-CA-C	-5.67	100.43	109.04
1	C	123	ARG	O-C-N	-5.67	114.47	122.06
2	B	32	GLU	O-C-N	-5.66	116.20	122.09
1	C	284	LEU	CA-C-O	-5.66	114.41	120.92
2	B	512	LYS	CA-CB-CG	5.66	125.42	114.10
1	A	75	TYR	CA-C-N	5.66	128.43	120.28
1	A	75	TYR	C-N-CA	5.66	128.43	120.28
1	A	357	GLN	O-C-N	-5.66	114.17	122.43
2	B	410	ARG	CB-CG-CD	5.66	124.32	111.30
2	B	503	ARG	CA-C-N	5.66	128.43	120.28
2	B	503	ARG	C-N-CA	5.66	128.43	120.28
1	C	554	LYS	O-C-N	5.66	128.14	122.08
2	D	69	GLY	CA-C-O	-5.66	110.72	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	637	ALA	CA-C-N	5.66	131.88	121.70
2	B	637	ALA	C-N-CA	5.66	131.88	121.70
1	C	257	ALA	N-CA-C	5.66	117.12	111.07
1	A	639	GLU	CB-CA-C	5.65	121.09	110.63
2	B	355	ALA	N-CA-C	-5.65	102.53	110.50
2	D	280	ILE	CA-C-N	5.65	131.97	122.87
2	D	280	ILE	C-N-CA	5.65	131.97	122.87
1	A	545	VAL	CA-C-N	5.65	126.21	119.94
1	A	545	VAL	C-N-CA	5.65	126.21	119.94
2	D	370	PRO	N-CA-CB	5.65	108.28	103.19
1	C	393	GLU	N-CA-C	5.65	120.45	113.50
1	C	443	LYS	CA-CB-CG	5.65	125.39	114.10
2	D	488	LEU	CA-C-O	-5.65	115.30	120.95
1	A	715	ALA	O-C-N	-5.64	116.00	122.09
1	C	264	VAL	N-CA-C	-5.64	105.00	110.42
1	C	724	ALA	CA-C-O	-5.64	113.88	120.20
1	A	660	GLY	O-C-N	-5.64	116.30	122.84
1	A	696	LEU	CA-C-O	-5.64	114.87	120.90
1	A	537	ASP	CA-C-O	-5.64	114.90	120.82
1	A	569	VAL	N-CA-CB	5.64	117.61	111.41
1	C	39	GLU	CA-CB-CG	5.64	125.37	114.10
1	C	122	HIS	N-CA-C	5.64	117.87	111.11
1	C	203	GLU	N-CA-CB	5.64	118.24	110.07
1	A	205	MET	CA-C-O	-5.63	114.90	120.82
2	B	428	GLY	N-CA-C	-5.63	106.39	112.08
1	A	101	PHE	CB-CA-C	5.63	119.72	110.88
1	A	362	SER	N-CA-CB	5.63	121.49	111.69
1	A	414	TRP	CA-C-N	5.63	128.10	120.44
1	A	414	TRP	C-N-CA	5.63	128.10	120.44
2	D	555	GLU	N-CA-C	-5.63	105.05	111.07
2	D	306	ARG	O-C-N	5.63	127.88	122.03
2	D	291	PHE	N-CA-C	5.63	118.35	111.82
2	D	467	PRO	N-CA-CB	5.63	109.16	103.25
1	C	452	ARG	CA-C-N	5.62	128.61	120.79
1	C	452	ARG	C-N-CA	5.62	128.61	120.79
1	C	281	ALA	N-CA-CB	5.62	119.14	110.43
2	D	494	SER	N-CA-CB	-5.62	102.32	110.47
1	A	711	ILE	O-C-N	-5.62	116.82	120.42
2	B	126	LEU	CA-C-N	5.62	128.12	120.54
2	B	126	LEU	C-N-CA	5.62	128.12	120.54
1	C	389	PHE	CA-CB-CG	-5.62	108.18	113.80
1	C	527	PRO	N-CA-CB	5.62	108.68	103.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	684	VAL	CA-CB-CG2	5.62	119.95	110.40
2	B	181	SER	O-C-N	-5.62	116.07	122.08
1	C	191	GLN	OE1-CD-NE2	-5.62	116.98	122.60
2	D	567	LEU	CA-C-O	5.61	127.09	120.69
2	B	363	PHE	N-CA-C	5.61	119.38	112.54
2	B	391	ASN	O-C-N	-5.61	115.05	122.40
2	D	491	HIS	N-CA-CB	5.61	120.24	110.81
1	A	650	HIS	CA-C-O	5.61	126.16	119.60
1	A	517	TRP	CA-CB-CG	-5.61	102.95	113.60
1	C	226	ALA	CA-C-O	-5.61	114.90	121.07
2	D	269	GLN	O-C-N	-5.61	113.39	122.42
1	C	37	ALA	N-CA-C	5.61	118.14	110.24
2	D	111	ALA	N-CA-C	5.61	118.37	109.96
1	C	602	LEU	CB-CA-C	5.60	119.58	110.22
2	B	82	PRO	CB-CA-C	-5.60	103.89	111.12
1	C	129	ASN	CA-C-N	5.60	125.07	119.24
1	C	129	ASN	C-N-CA	5.60	125.07	119.24
2	D	346	ALA	CA-C-O	-5.60	114.94	120.82
1	A	120	PRO	O-C-N	-5.60	115.51	122.23
1	A	69	PRO	CA-C-N	5.60	130.07	122.07
1	A	69	PRO	C-N-CA	5.60	130.07	122.07
1	A	153	PHE	CA-CB-CG	-5.60	108.20	113.80
1	C	288	TRP	CB-CA-C	-5.60	99.64	109.71
2	B	417	TRP	N-CA-C	-5.60	104.87	110.97
2	B	573	VAL	CA-C-O	-5.59	114.43	120.47
1	C	320	PRO	CA-C-O	5.59	126.30	118.86
2	D	183	TYR	O-C-N	-5.59	116.31	122.07
1	A	190	GLU	CB-CG-CD	5.59	122.11	112.60
2	D	460	ILE	N-CA-CB	5.59	119.26	112.10
1	C	207	ARG	N-CA-CB	-5.59	101.69	110.30
1	C	604	LYS	CA-C-O	5.59	127.07	120.70
2	D	614	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	209	GLY	CA-C-N	5.59	134.65	123.20
2	B	209	GLY	C-N-CA	5.59	134.65	123.20
1	C	551	ALA	N-CA-C	5.59	118.90	111.75
1	C	439	LYS	O-C-N	-5.58	114.75	122.46
2	B	112	LEU	CA-C-O	5.58	126.85	120.54
1	C	724	ALA	CA-C-N	5.58	128.22	120.63
1	C	724	ALA	C-N-CA	5.58	128.22	120.63
1	A	404	SER	CA-C-O	5.58	127.04	120.96
2	D	133	VAL	CB-CA-C	-5.58	103.85	111.33
1	A	527	PRO	CA-C-N	5.58	130.04	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PRO	C-N-CA	5.58	130.04	120.72
1	C	10	VAL	CA-C-N	-5.58	114.34	122.65
1	C	10	VAL	C-N-CA	-5.58	114.34	122.65
1	A	211	ILE	CA-C-N	5.58	139.33	121.98
1	A	211	ILE	C-N-CA	5.58	139.33	121.98
1	A	347	ARG	NE-CZ-NH1	5.58	127.08	121.50
2	D	601	GLU	O-C-N	-5.58	115.14	122.39
1	A	158	LEU	N-CA-C	5.58	119.56	112.87
2	B	142	PRO	CA-C-N	5.58	131.71	122.73
2	B	142	PRO	C-N-CA	5.58	131.71	122.73
1	C	664	LEU	CB-CA-C	-5.58	100.50	110.70
2	B	405	VAL	CB-CA-C	5.57	119.67	112.14
2	D	334	GLU	O-C-N	-5.57	116.28	122.86
2	D	380	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	A	401	ASP	CB-CA-C	5.57	121.15	110.17
2	B	339	ASN	CB-CG-ND2	-5.57	108.04	116.40
1	C	400	ILE	CA-C-N	5.57	135.40	121.80
1	C	400	ILE	C-N-CA	5.57	135.40	121.80
1	A	71	VAL	N-CA-CB	5.57	117.07	110.55
1	C	377	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	356	THR	O-C-N	-5.57	114.87	122.33
1	A	569	VAL	O-C-N	5.57	126.93	121.98
1	A	574	VAL	N-CA-C	-5.57	97.87	106.72
1	C	517	TRP	CA-CB-CG	-5.57	103.03	113.60
2	D	494	SER	N-CA-C	5.57	119.70	113.02
1	C	639	GLU	O-C-N	-5.56	115.43	122.27
2	D	433	VAL	CA-C-N	5.56	128.19	120.29
2	D	433	VAL	C-N-CA	5.56	128.19	120.29
2	B	314	ASP	O-C-N	-5.56	116.39	123.06
2	B	506	SER	CA-C-N	5.56	128.87	120.75
2	B	506	SER	C-N-CA	5.56	128.87	120.75
1	C	138	MET	N-CA-C	5.56	119.23	112.23
1	C	398	ARG	CA-CB-CG	5.56	125.22	114.10
2	D	533	PRO	CA-C-N	5.56	128.05	120.77
2	D	533	PRO	C-N-CA	5.56	128.05	120.77
1	A	327	THR	N-CA-CB	-5.56	102.20	111.20
2	B	472	ARG	CD-NE-CZ	5.56	132.18	124.40
2	B	97	THR	CA-CB-OG1	-5.56	101.27	109.60
2	B	544	GLN	N-CA-C	5.56	116.69	108.86
1	C	233	PRO	N-CA-CB	5.56	109.41	103.52
1	C	348	THR	CA-C-N	5.56	127.66	120.44
1	C	348	THR	C-N-CA	5.56	127.66	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	560	THR	N-CA-C	-5.55	99.97	109.24
1	A	454	GLN	OE1-CD-NE2	-5.55	117.05	122.60
2	B	578	GLY	CA-C-N	5.55	128.51	120.79
2	B	578	GLY	C-N-CA	5.55	128.51	120.79
1	C	215	GLN	CA-C-O	5.55	127.77	120.16
1	C	207	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	C	215	GLN	O-C-N	-5.55	114.94	121.32
1	A	594	GLU	CA-CB-CG	5.55	125.20	114.10
2	B	211	GLU	CA-C-O	5.55	125.35	120.19
1	C	533	LYS	CG-CD-CE	5.55	124.06	111.30
1	C	94	THR	N-CA-C	5.54	119.01	110.42
1	C	100	ALA	CA-C-N	5.54	127.64	120.44
1	C	100	ALA	C-N-CA	5.54	127.64	120.44
2	D	245	GLY	CA-C-O	-5.54	113.41	118.95
2	D	438	VAL	CB-CA-C	5.54	119.30	112.04
2	B	148	GLU	N-CA-CB	5.54	118.26	110.12
1	C	70	PHE	N-CA-C	5.54	122.60	110.80
1	C	332	SER	N-CA-C	5.54	117.73	109.59
1	A	79	TYR	CB-CG-CD2	-5.54	112.49	120.80
1	A	278	ASP	O-C-N	-5.54	115.07	122.43
1	A	623	ASP	O-C-N	-5.54	115.19	122.39
2	B	538	ALA	N-CA-C	5.54	119.78	113.19
2	D	633	ILE	CA-C-N	5.54	132.40	122.38
2	D	633	ILE	C-N-CA	5.54	132.40	122.38
1	A	369	ASP	CA-C-N	5.53	132.11	121.54
1	A	369	ASP	C-N-CA	5.53	132.11	121.54
2	B	568	CYS	CA-C-O	-5.53	114.38	120.36
2	D	426	LEU	CB-CA-C	-5.53	100.85	110.09
2	D	565	ALA	O-C-N	5.53	129.87	123.17
2	D	162	THR	CA-CB-OG1	-5.53	101.30	109.60
2	D	67	VAL	CA-C-N	5.53	132.10	121.54
2	D	67	VAL	C-N-CA	5.53	132.10	121.54
1	A	158	LEU	CA-C-N	5.53	132.34	122.06
1	A	158	LEU	C-N-CA	5.53	132.34	122.06
1	C	221	ILE	CA-CB-CG1	5.53	119.80	110.40
2	D	185	ARG	N-CA-C	5.53	122.57	110.80
1	C	581	GLU	CA-C-O	-5.52	115.02	120.82
1	C	97	GLU	O-C-N	-5.52	116.38	122.07
1	A	556	PHE	N-CA-CB	-5.52	102.41	110.47
2	B	316	ASP	CA-C-O	5.52	125.44	119.15
1	A	131	ARG	N-CA-CB	-5.52	101.23	110.39
2	B	367	LEU	CB-CA-C	-5.52	100.78	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	ASP	O-C-N	-5.52	116.56	122.85
2	D	110	ARG	CD-NE-CZ	5.51	132.12	124.40
1	C	436	ALA	O-C-N	-5.51	116.28	122.12
1	C	436	ALA	CB-CA-C	5.51	119.94	110.79
2	D	490	TRP	CA-CB-CG	5.51	124.06	113.60
1	A	420	ALA	CA-C-N	5.50	128.21	120.28
1	A	420	ALA	C-N-CA	5.50	128.21	120.28
1	A	677	ARG	O-C-N	-5.50	116.42	121.37
1	C	280	PHE	N-CA-CB	-5.50	103.11	111.15
2	B	184	GLU	O-C-N	-5.50	116.40	122.07
2	D	75	MET	CA-C-O	5.50	127.05	120.28
1	A	635	GLN	CA-CB-CG	5.50	125.10	114.10
1	A	636	THR	N-CA-C	-5.50	102.14	110.39
1	C	117	PHE	O-C-N	-5.50	116.75	123.19
1	C	172	LEU	CA-C-N	5.50	125.16	119.05
1	C	172	LEU	C-N-CA	5.50	125.16	119.05
1	C	699	ASP	N-CA-CB	-5.50	102.02	110.44
1	C	196	ILE	CA-C-N	-5.50	113.39	120.65
1	C	196	ILE	C-N-CA	-5.50	113.39	120.65
2	D	226	LYS	CA-CB-CG	5.50	125.10	114.10
2	B	141	ASP	CA-C-N	5.50	125.15	119.05
2	B	141	ASP	C-N-CA	5.50	125.15	119.05
2	B	381	ASN	CA-C-O	-5.50	113.89	120.10
2	B	438	VAL	CA-C-O	-5.50	115.55	121.27
1	A	184	GLU	O-C-N	-5.49	115.25	122.39
1	A	531	LEU	CA-C-O	-5.49	114.73	120.55
2	B	28	PRO	N-CA-CB	5.49	108.20	103.31
1	C	641	ALA	O-C-N	-5.49	116.41	122.07
2	B	181	SER	CA-C-N	5.49	127.68	120.60
2	B	181	SER	C-N-CA	5.49	127.68	120.60
2	B	455	ASN	CA-C-O	5.49	125.98	119.56
2	D	52	GLN	CA-CB-CG	5.49	125.07	114.10
1	A	332	SER	CA-C-N	5.48	126.07	119.98
1	A	332	SER	C-N-CA	5.48	126.07	119.98
1	A	236	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	C	146	ILE	CA-C-O	5.48	126.43	120.57
2	D	40	GLU	CB-CA-C	-5.48	101.69	110.79
1	A	314	GLN	CA-C-N	5.48	132.03	121.18
1	A	314	GLN	C-N-CA	5.48	132.03	121.18
1	A	501	ALA	CA-C-O	-5.48	115.07	120.82
2	D	254	TRP	CB-CA-C	5.48	120.76	110.63
2	D	580	GLU	CA-C-N	5.48	127.66	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	580	GLU	C-N-CA	5.48	127.66	120.60
1	A	410	GLU	CB-CG-CD	5.47	121.91	112.60
1	A	591	GLU	CA-C-N	5.47	127.62	120.28
1	A	591	GLU	C-N-CA	5.47	127.62	120.28
2	B	185	ARG	O-C-N	-5.47	115.31	122.59
1	C	573	GLU	CA-C-N	-5.47	112.11	121.97
1	C	573	GLU	C-N-CA	-5.47	112.11	121.97
2	D	341	LEU	N-CA-C	-5.47	105.39	111.36
1	A	484	ASP	CA-C-O	-5.47	114.93	120.84
2	D	77	ARG	CA-C-O	5.47	127.66	120.16
1	A	69	PRO	O-C-N	-5.47	110.71	121.10
1	C	17	VAL	CB-CA-C	-5.47	104.59	111.04
1	C	140	GLY	CA-C-N	-5.47	113.31	120.91
1	C	140	GLY	C-N-CA	-5.47	113.31	120.91
2	D	23	LEU	CA-C-O	5.47	125.42	119.40
2	D	537	ILE	CA-C-O	-5.47	115.58	121.27
2	B	265	ALA	CA-C-N	5.47	127.61	120.28
2	B	265	ALA	C-N-CA	5.47	127.61	120.28
2	D	134	THR	N-CA-C	5.47	120.22	113.50
1	A	388	LEU	N-CA-C	-5.47	105.24	111.14
2	B	463	VAL	CA-C-N	-5.47	113.14	122.11
2	B	463	VAL	C-N-CA	-5.47	113.14	122.11
1	A	255	GLU	N-CA-C	-5.46	105.23	111.07
1	A	262	ASP	CA-C-N	5.46	126.16	119.99
1	A	262	ASP	C-N-CA	5.46	126.16	119.99
1	A	367	SER	CA-C-O	5.46	128.17	121.56
1	A	437	ILE	CB-CA-C	5.46	119.56	112.24
1	A	59	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	205	ALA	O-C-N	-5.46	116.24	122.08
2	B	485	ARG	CA-C-O	-5.45	114.73	121.11
1	A	94	THR	N-CA-C	5.45	118.87	110.42
1	A	361	GLN	CA-CB-CG	5.45	125.00	114.10
2	B	55	PHE	CA-CB-CG	-5.45	108.35	113.80
1	C	356	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	448	GLU	CA-C-N	5.45	127.58	120.28
1	A	448	GLU	C-N-CA	5.45	127.58	120.28
2	B	273	ALA	N-CA-CB	5.45	118.72	110.28
2	D	340	ILE	CA-C-N	5.45	128.03	120.29
2	D	340	ILE	C-N-CA	5.45	128.03	120.29
1	A	339	GLN	CA-CB-CG	5.45	124.99	114.10
1	C	549	SER	CA-C-N	5.45	127.85	120.44
1	C	549	SER	C-N-CA	5.45	127.85	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	164	VAL	O-C-N	-5.45	117.30	123.18
2	D	228	SER	CA-C-O	5.45	127.19	120.87
1	A	339	GLN	O-C-N	-5.45	116.30	123.16
1	C	579	GLU	CA-CB-CG	5.45	124.99	114.10
2	D	163	LYS	CA-C-O	-5.44	114.84	121.05
2	B	625	ASP	O-C-N	-5.44	116.37	122.03
1	C	188	LYS	CA-C-O	5.44	126.24	120.64
2	D	611	LYS	CA-C-O	-5.44	115.08	120.90
1	A	220	ILE	CA-C-N	5.44	127.89	120.77
1	A	220	ILE	C-N-CA	5.44	127.89	120.77
1	A	380	ALA	CA-C-N	5.44	127.51	120.44
1	A	380	ALA	C-N-CA	5.44	127.51	120.44
1	C	247	GLU	N-CA-C	5.44	117.96	111.71
1	C	446	ILE	CA-C-N	5.44	128.01	120.29
1	C	446	ILE	C-N-CA	5.44	128.01	120.29
1	C	610	HIS	N-CA-C	5.44	117.58	109.59
2	B	261	GLU	CA-C-O	-5.43	115.11	120.82
1	C	469	LYS	CA-C-N	5.43	130.08	122.36
1	C	469	LYS	C-N-CA	5.43	130.08	122.36
1	A	314	GLN	N-CA-C	-5.43	105.44	111.36
1	C	583	ALA	CA-C-N	5.43	127.50	120.44
1	C	583	ALA	C-N-CA	5.43	127.50	120.44
1	A	248	ALA	N-CA-CB	5.43	119.41	110.39
1	C	38	TRP	CA-C-O	-5.43	114.45	120.70
1	A	261	ALA	N-CA-C	-5.43	105.52	111.82
1	A	466	GLY	O-C-N	-5.43	116.14	122.60
2	B	214	LEU	N-CA-CB	-5.43	102.33	110.91
1	C	163	VAL	O-C-N	-5.43	117.40	123.26
1	C	217	SER	O-C-N	-5.43	116.48	122.07
2	D	191	LYS	N-CA-C	5.43	119.39	112.87
1	A	627	ASP	N-CA-C	-5.43	98.38	107.99
2	B	46	GLY	CA-C-N	5.43	131.89	122.28
2	B	46	GLY	C-N-CA	5.43	131.89	122.28
2	B	610	GLU	CA-C-N	5.43	128.10	120.28
2	B	610	GLU	C-N-CA	5.43	128.10	120.28
1	C	194	GLY	O-C-N	-5.43	118.72	123.88
1	C	639	GLU	CB-CA-C	-5.43	100.25	110.67
1	A	677	ARG	CA-CB-CG	5.43	124.95	114.10
2	B	627	LEU	CA-C-O	-5.43	114.67	120.42
2	D	282	PHE	CA-C-O	-5.43	114.50	120.36
2	D	585	LEU	O-C-N	-5.43	116.27	122.08
1	A	80	ALA	N-CA-C	-5.42	105.37	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	SER	O-C-N	-5.42	116.55	123.06
2	D	479	PHE	CA-C-N	5.42	125.43	119.90
2	D	479	PHE	C-N-CA	5.42	125.43	119.90
1	A	133	ALA	O-C-N	-5.42	115.38	122.59
1	A	256	MET	O-C-N	-5.42	116.28	122.08
2	D	50	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	669	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	A	74	PRO	O-C-N	-5.41	114.96	122.27
1	A	161	MET	CB-CG-SD	5.41	128.94	112.70
2	B	47	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	C	715	ALA	CA-C-O	5.41	126.69	120.90
2	D	321	ARG	O-C-N	5.41	130.26	123.12
2	D	429	MET	CA-C-N	5.41	127.48	120.44
2	D	429	MET	C-N-CA	5.41	127.48	120.44
1	C	73	GLY	N-CA-C	-5.41	101.30	112.34
2	D	542	THR	O-C-N	-5.41	116.50	121.37
2	B	388	GLU	CB-CG-CD	5.41	121.80	112.60
1	C	311	LEU	CA-C-O	-5.41	115.32	121.00
2	B	146	ALA	N-CA-C	-5.41	102.83	110.29
2	B	165	GLU	CA-C-O	-5.41	114.78	121.11
2	B	182	VAL	O-C-N	-5.41	116.53	121.94
1	A	541	ALA	N-CA-C	5.40	119.62	113.19
1	C	443	LYS	O-C-N	-5.40	115.90	122.22
1	C	667	ALA	N-CA-C	-5.40	105.47	111.36
1	C	177	LEU	CA-C-O	-5.40	114.00	120.10
1	A	152	LEU	CB-CA-C	-5.40	101.67	110.85
1	C	589	GLU	CA-C-O	5.40	126.97	120.92
2	D	265	ALA	CA-C-O	-5.40	113.24	119.61
1	A	163	VAL	CA-C-N	-5.40	114.61	122.65
1	A	163	VAL	C-N-CA	-5.40	114.61	122.65
2	B	239	ASN	O-C-N	-5.40	115.90	122.22
1	C	129	ASN	N-CA-C	-5.40	99.67	109.44
2	B	420	PHE	N-CA-C	-5.40	105.05	111.69
1	C	205	MET	O-C-N	-5.40	116.00	122.15
2	D	147	PRO	N-CA-CB	5.40	109.41	103.26
2	B	112	LEU	O-C-N	-5.39	117.07	123.22
1	A	251	THR	CA-C-N	5.39	128.91	120.82
1	A	251	THR	C-N-CA	5.39	128.91	120.82
1	A	268	ARG	CB-CG-CD	-5.39	98.89	111.30
2	D	395	VAL	N-CA-CB	5.39	119.39	111.52
1	C	99	ASN	O-C-N	-5.39	116.52	122.07
1	C	174	ILE	CA-C-N	5.39	127.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ILE	C-N-CA	5.39	127.45	120.44
1	A	312	VAL	CA-C-N	5.39	129.22	120.60
1	A	312	VAL	C-N-CA	5.39	129.22	120.60
1	C	247	GLU	CA-C-N	5.39	129.84	120.68
1	C	247	GLU	C-N-CA	5.39	129.84	120.68
2	D	424	GLU	N-CA-C	-5.39	105.31	111.07
2	D	558	LYS	CA-C-N	5.39	127.50	120.28
2	D	558	LYS	C-N-CA	5.39	127.50	120.28
2	B	396	ASN	CB-CA-C	-5.38	101.06	109.84
2	D	449	ARG	O-C-N	-5.38	116.41	122.12
1	A	467	VAL	CA-C-N	-5.38	114.12	122.67
1	A	467	VAL	C-N-CA	-5.38	114.12	122.67
2	B	23	LEU	CA-C-N	5.38	127.93	120.29
2	B	23	LEU	C-N-CA	5.38	127.93	120.29
2	B	290	GLN	N-CA-C	5.38	116.83	111.07
1	A	271	GLU	O-C-N	-5.38	116.42	122.12
2	B	201	PRO	O-C-N	-5.38	115.78	122.23
1	A	652	VAL	CB-CA-C	-5.38	104.44	111.81
2	D	64	VAL	CA-C-N	5.38	130.58	123.00
2	D	64	VAL	C-N-CA	5.38	130.58	123.00
2	B	601	GLU	CA-CB-CG	-5.38	103.35	114.10
1	C	128	ASP	CA-C-O	-5.37	112.93	119.43
1	C	61	LEU	N-CA-C	5.37	117.89	111.71
2	D	367	LEU	CB-CA-C	-5.37	99.73	110.42
1	A	430	VAL	CA-C-O	5.37	126.17	120.26
1	C	720	LYS	O-C-N	-5.37	116.43	122.12
2	D	617	LEU	N-CA-CB	5.37	119.18	110.43
1	A	407	ALA	CA-C-O	-5.37	113.80	119.97
2	B	443	ASP	CA-C-N	5.37	127.42	120.44
2	B	443	ASP	C-N-CA	5.37	127.42	120.44
2	B	631	LEU	N-CA-C	-5.37	105.51	111.36
2	D	318	ARG	CG-CD-NE	-5.36	100.20	112.00
2	B	48	PRO	N-CA-CB	5.36	108.28	103.08
1	C	295	PHE	N-CA-CB	5.36	118.47	110.22
1	C	512	LEU	CA-C-N	5.36	127.46	120.28
1	C	512	LEU	C-N-CA	5.36	127.46	120.28
1	C	651	VAL	N-CA-C	5.36	116.38	108.45
2	D	65	HIS	CB-CG-CD2	5.36	138.17	131.20
2	D	68	ASP	O-C-N	-5.36	115.46	122.59
1	A	527	PRO	CB-CA-C	-5.36	103.85	112.21
1	A	717	SER	CA-C-N	5.36	129.66	120.71
1	A	717	SER	C-N-CA	5.36	129.66	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	PRO	CB-CA-C	-5.36	104.24	111.85
1	A	370	GLU	O-C-N	-5.36	115.47	122.59
2	B	331	LEU	O-C-N	-5.36	116.22	122.81
1	C	68	PRO	O-C-N	-5.36	115.14	121.46
2	D	510	ARG	CA-C-O	5.36	125.74	120.17
2	D	601	GLU	CA-C-O	5.35	125.97	119.49
1	A	461	ARG	CA-C-O	-5.35	115.20	120.82
1	A	702	VAL	CA-CB-CG2	5.35	119.50	110.40
2	B	490	TRP	CA-C-O	5.35	126.21	120.32
2	D	308	GLY	N-CA-C	5.35	125.86	113.18
1	C	382	ILE	CA-C-O	-5.35	115.50	121.17
1	A	598	PRO	N-CA-C	-5.35	102.80	111.03
2	B	228	SER	CA-C-N	5.35	125.43	119.87
2	B	228	SER	C-N-CA	5.35	125.43	119.87
1	A	521	ASN	CB-CA-C	-5.35	102.42	110.87
1	C	65	ALA	N-CA-CB	5.34	117.90	109.83
1	C	140	GLY	O-C-N	5.34	129.16	123.81
1	A	23	ARG	CA-C-N	5.34	127.88	120.29
1	A	23	ARG	C-N-CA	5.34	127.88	120.29
1	A	267	ILE	CA-C-O	5.34	126.83	121.17
2	B	425	LYS	CA-C-O	-5.34	114.89	120.55
1	C	54	VAL	CA-CB-CG2	5.34	119.48	110.40
1	C	672	LEU	O-C-N	-5.34	116.46	122.12
2	D	335	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	248	ALA	O-C-N	-5.34	115.28	122.43
1	C	200	ILE	CA-C-O	5.34	126.02	120.25
2	D	551	ALA	N-CA-C	-5.34	104.51	111.02
1	C	358	GLY	O-C-N	-5.33	115.77	122.70
1	A	159	ASP	CA-C-N	5.33	130.60	122.23
1	A	159	ASP	C-N-CA	5.33	130.60	122.23
2	B	49	PRO	N-CA-CB	5.33	108.85	103.25
1	C	633	LEU	CA-C-N	5.33	131.42	123.05
1	C	633	LEU	C-N-CA	5.33	131.42	123.05
1	A	495	LYS	CG-CD-CE	5.33	123.56	111.30
2	B	119	LYS	CB-CA-C	-5.33	102.48	110.90
1	C	491	GLU	O-C-N	-5.33	116.47	122.12
2	B	459	PRO	CA-C-N	5.32	130.46	123.11
2	B	459	PRO	C-N-CA	5.32	130.46	123.11
1	C	673	ASP	N-CA-C	-5.32	105.12	111.03
2	D	109	VAL	CA-C-O	-5.32	114.46	120.74
2	D	265	ALA	O-C-N	-5.32	115.41	122.33
2	D	383	GLY	CA-C-O	5.32	125.78	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASP	CA-C-N	5.32	132.29	122.92
1	A	62	ASP	C-N-CA	5.32	132.29	122.92
2	B	322	GLN	CB-CG-CD	5.32	121.65	112.60
1	C	391	GLN	CG-CD-OE1	5.32	131.44	120.80
2	B	512	LYS	O-C-N	-5.32	117.10	123.27
1	C	154	ALA	CA-C-N	5.32	130.59	121.07
1	C	154	ALA	C-N-CA	5.32	130.59	121.07
1	C	590	PHE	CA-C-N	5.32	127.40	120.28
1	C	590	PHE	C-N-CA	5.32	127.40	120.28
2	B	245	GLY	CA-C-N	-5.32	112.57	121.39
2	B	245	GLY	C-N-CA	-5.32	112.57	121.39
2	B	352	VAL	CB-CA-C	5.32	120.87	112.26
1	C	65	ALA	N-CA-C	-5.32	102.52	110.23
1	C	603	ALA	CA-C-O	5.32	127.33	121.11
2	D	280	ILE	CA-C-O	5.32	125.97	120.39
1	A	43	GLN	CA-C-N	5.31	133.17	123.34
1	A	43	GLN	C-N-CA	5.31	133.17	123.34
1	A	566	ILE	CA-C-O	-5.31	116.76	121.97
1	C	634	PHE	CA-C-N	5.31	129.28	120.94
1	C	634	PHE	C-N-CA	5.31	129.28	120.94
2	D	109	VAL	N-CA-C	-5.31	100.67	108.54
2	D	582	ALA	N-CA-C	-5.31	105.38	111.07
1	C	401	ASP	CA-CB-CG	5.31	117.91	112.60
2	D	304	TRP	CA-C-N	5.31	127.66	120.38
2	D	304	TRP	C-N-CA	5.31	127.66	120.38
2	B	611	LYS	O-C-N	-5.31	116.01	122.22
1	C	485	ASN	OD1-CG-ND2	5.31	127.91	122.60
2	D	456	ARG	CA-C-O	5.31	126.94	120.57
2	D	463	VAL	O-C-N	5.31	129.21	122.57
2	D	632	ASP	CA-C-N	5.31	131.53	121.97
2	D	632	ASP	C-N-CA	5.31	131.53	121.97
2	D	52	GLN	N-CA-C	5.31	117.89	109.24
1	A	180	VAL	O-C-N	-5.30	116.64	121.94
1	C	201	LEU	O-C-N	-5.30	116.50	122.12
1	C	590	PHE	CA-C-O	-5.30	115.22	120.90
1	A	703	GLU	CA-CB-CG	5.30	124.70	114.10
1	A	75	TYR	O-C-N	-5.30	116.99	123.19
1	A	711	ILE	CA-C-N	5.30	124.48	118.97
1	A	711	ILE	C-N-CA	5.30	124.48	118.97
1	A	301	LEU	CA-C-N	5.30	129.56	120.71
1	A	301	LEU	C-N-CA	5.30	129.56	120.71
1	A	475	GLU	CB-CA-C	-5.29	101.19	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	220	TRP	CA-C-O	-5.29	115.23	120.90
2	B	340	ILE	N-CA-CB	5.29	118.52	110.58
2	B	506	SER	CA-CB-OG	5.29	121.68	111.10
1	C	460	GLY	N-CA-C	-5.29	107.49	114.95
2	D	262	TYR	N-CA-CB	-5.29	102.07	110.22
1	A	555	VAL	CA-C-O	-5.29	114.36	119.92
2	D	179	LEU	CA-C-O	-5.29	115.27	120.82
2	B	315	GLU	CA-CB-CG	5.29	124.67	114.10
1	A	718	LEU	CB-CA-C	-5.29	101.91	110.79
1	C	350	ILE	CA-C-N	5.29	127.36	120.28
1	C	350	ILE	C-N-CA	5.29	127.36	120.28
2	D	113	HIS	CA-C-N	5.29	129.85	121.18
2	D	113	HIS	C-N-CA	5.29	129.85	121.18
1	A	349	CYS	CA-C-N	5.28	127.70	120.46
1	A	349	CYS	C-N-CA	5.28	127.70	120.46
1	A	438	GLU	CA-C-O	-5.28	114.13	120.10
2	B	277	PHE	O-C-N	-5.28	116.59	122.09
2	B	362	PRO	CA-C-O	-5.28	115.35	121.95
1	C	619	THR	CA-C-N	5.28	129.66	120.68
1	C	619	THR	C-N-CA	5.28	129.66	120.68
1	A	403	TRP	CA-C-N	5.28	128.60	121.05
1	A	403	TRP	C-N-CA	5.28	128.60	121.05
1	C	385	ASN	CA-C-O	-5.28	114.93	120.63
2	D	21	LEU	CA-C-O	5.28	126.62	120.49
2	D	616	ARG	N-CA-C	5.28	118.17	109.72
1	A	53	ASP	O-C-N	-5.28	116.13	122.15
1	C	152	LEU	CA-C-N	5.28	131.25	122.54
1	C	152	LEU	C-N-CA	5.28	131.25	122.54
1	C	694	ASP	CA-C-O	5.28	126.10	120.24
1	C	543	ALA	CA-C-O	-5.28	115.58	121.81
1	C	658	ALA	N-CA-C	5.28	119.41	112.92
2	D	197	LEU	CB-CA-C	5.28	118.90	109.29
1	A	253	ASP	CA-CB-CG	5.28	117.88	112.60
2	B	179	LEU	CA-C-O	-5.28	115.28	120.82
2	D	477	LYS	N-CA-C	-5.27	101.97	109.62
1	A	550	ASP	N-CA-C	-5.27	105.43	111.07
1	A	689	PRO	N-CA-CB	5.27	108.00	103.31
2	B	419	GLU	O-C-N	-5.27	115.37	122.43
1	C	89	TYR	CA-CB-CG	5.27	123.38	113.90
1	C	423	HIS	O-C-N	-5.27	116.61	122.09
1	C	545	VAL	CA-C-N	5.27	125.68	119.94
1	C	545	VAL	C-N-CA	5.27	125.68	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	655	SER	CA-C-O	5.27	125.93	120.40
2	D	61	ARG	CA-C-O	-5.27	114.30	120.20
2	D	164	VAL	CB-CA-C	5.27	118.47	110.62
1	A	678	PRO	CA-N-CD	-5.27	104.63	112.00
1	C	268	ARG	CG-CD-NE	-5.27	100.41	112.00
2	B	334	GLU	CA-C-O	5.26	127.05	121.05
1	A	661	HIS	CB-CA-C	5.26	119.47	110.74
1	A	668	LEU	N-CA-CB	5.26	117.70	110.07
1	C	478	LEU	CA-C-O	5.26	125.93	120.30
2	D	28	PRO	N-CA-CB	5.26	107.74	103.32
2	B	64	VAL	CA-C-N	5.26	130.41	123.00
2	B	64	VAL	C-N-CA	5.26	130.41	123.00
2	D	537	ILE	N-CA-CB	5.26	116.35	110.51
2	D	605	ASP	CA-CB-CG	-5.26	107.34	112.60
2	B	24	ALA	N-CA-C	-5.26	105.63	111.36
2	B	207	LEU	CA-C-O	-5.26	113.92	119.97
1	C	243	TYR	N-CA-CB	5.26	117.81	109.82
2	B	520	THR	O-C-N	-5.25	116.53	122.68
2	D	157	VAL	N-CA-C	5.25	116.31	108.54
2	D	396	ASN	N-CA-C	-5.25	101.41	109.76
2	B	225	ALA	O-C-N	-5.25	115.50	122.33
2	D	258	THR	CA-C-O	-5.25	114.98	120.55
2	D	546	GLU	CA-C-O	5.25	128.06	122.13
1	C	295	PHE	CA-C-O	-5.25	114.17	120.10
1	A	723	ARG	NH1-CZ-NH2	-5.25	112.48	119.30
1	C	590	PHE	CB-CA-C	-5.25	102.42	110.81
1	A	588	GLU	CA-C-O	-5.24	115.31	120.82
2	D	550	THR	CA-C-N	5.24	128.08	120.79
2	D	550	THR	C-N-CA	5.24	128.08	120.79
2	D	587	ALA	CA-C-N	5.24	129.07	120.63
2	D	587	ALA	C-N-CA	5.24	129.07	120.63
2	B	574	TYR	CA-C-N	5.24	127.57	120.65
2	B	574	TYR	C-N-CA	5.24	127.57	120.65
1	C	513	ASP	O-C-N	-5.24	116.56	122.12
1	A	202	LYS	O-C-N	-5.24	115.82	122.27
1	A	525	LYS	N-CA-C	-5.24	106.66	113.16
2	D	275	GLU	CA-C-N	5.24	127.76	120.63
2	D	275	GLU	C-N-CA	5.24	127.76	120.63
1	A	27	GLU	O-C-N	-5.24	116.57	122.12
1	A	546	GLY	CA-C-O	-5.24	115.34	121.00
1	C	44	ILE	CB-CG1-CD1	5.24	124.80	113.80
2	D	82	PRO	CB-CA-C	-5.24	104.69	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	445	CYS	O-C-N	-5.24	115.86	122.20
2	B	96	GLY	CA-C-O	5.24	128.94	122.39
2	D	76	TYR	CA-CB-CG	-5.24	104.47	113.90
2	D	222	ARG	CA-CB-CG	5.24	124.57	114.10
1	C	45	PRO	O-C-N	-5.24	117.24	123.10
2	B	369	LEU	N-CA-C	-5.23	103.09	110.31
1	C	675	LEU	CA-C-O	5.23	125.61	119.28
1	A	463	PRO	CA-C-O	-5.23	115.28	121.67
2	D	521	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
1	A	493	LYS	CA-CB-CG	-5.23	103.64	114.10
2	B	618	PHE	CA-C-O	-5.23	115.68	121.33
1	C	271	GLU	O-C-N	-5.23	116.44	122.09
2	B	508	SER	CA-C-O	-5.23	112.95	119.38
1	A	63	THR	O-C-N	-5.23	116.36	123.10
1	A	538	ALA	CB-CA-C	-5.23	102.67	110.88
2	B	187	ASP	CA-C-N	5.23	137.21	122.21
2	B	187	ASP	C-N-CA	5.23	137.21	122.21
1	C	167	MET	CB-CA-C	5.23	118.68	109.80
2	B	527	ARG	CA-C-N	5.22	127.71	120.29
2	B	527	ARG	C-N-CA	5.22	127.71	120.29
2	D	206	ALA	CA-C-O	-5.22	115.31	120.90
2	D	202	ILE	O-C-N	-5.22	116.81	121.87
2	B	512	LYS	CB-CA-C	-5.22	97.97	109.56
2	B	536	HIS	O-C-N	-5.22	116.11	122.22
2	B	556	ALA	O-C-N	-5.22	116.50	122.08
1	C	236	ASN	CA-CB-CG	-5.22	107.38	112.60
1	C	690	GLU	N-CA-C	5.22	118.43	111.75
2	D	142	PRO	CB-CA-C	-5.22	104.07	112.21
2	B	130	GLU	O-C-N	-5.22	115.26	122.46
2	D	180	VAL	CA-C-O	-5.22	115.32	120.85
2	B	219	ASP	CA-C-O	5.21	127.97	120.51
1	C	580	VAL	CA-C-N	5.21	127.22	120.44
1	C	580	VAL	C-N-CA	5.21	127.22	120.44
2	D	594	TYR	N-CA-CB	5.21	120.00	111.08
2	D	599	PHE	O-C-N	-5.21	116.70	122.07
2	D	270	GLY	N-CA-C	5.21	122.78	115.43
1	A	715	ALA	N-CA-C	-5.21	105.51	111.14
2	B	256	LEU	O-C-N	-5.21	116.70	122.07
2	B	477	LYS	N-CA-C	-5.21	103.21	109.72
1	C	64	TYR	O-C-N	-5.21	116.59	123.21
2	D	515	LEU	CB-CA-C	5.21	118.63	110.19
1	C	159	ASP	CA-C-N	5.21	130.93	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ASP	C-N-CA	5.21	130.93	121.92
1	C	397	THR	O-C-N	-5.21	115.35	122.33
2	D	167	PHE	CB-CA-C	5.21	118.38	109.99
2	D	410	ARG	N-CA-C	-5.21	105.50	111.07
1	A	343	ASN	N-CA-C	-5.21	105.72	111.71
1	A	727	ASP	CA-C-O	5.21	129.10	121.86
2	B	172	GLN	CB-CA-C	5.21	119.05	110.88
2	B	569	SER	CA-C-O	-5.21	113.06	120.51
1	A	483	VAL	CB-CA-C	-5.21	104.08	111.21
2	B	143	ASP	CA-C-N	5.20	131.48	121.54
2	B	143	ASP	C-N-CA	5.20	131.48	121.54
2	D	201	PRO	N-CA-CB	5.20	108.80	103.23
1	A	347	ARG	CA-CB-CG	5.20	124.50	114.10
2	B	200	ASP	CA-C-O	5.20	127.29	120.16
2	B	495	GLU	CA-C-O	-5.20	114.91	120.42
2	B	534	VAL	O-C-N	-5.20	116.07	122.57
1	C	677	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	A	215	GLN	CB-CG-CD	5.20	121.44	112.60
2	D	438	VAL	N-CA-C	-5.20	105.78	110.82
1	C	117	PHE	N-CA-CB	-5.20	101.94	110.52
1	C	576	ASN	O-C-N	-5.20	115.45	122.41
1	C	185	GLN	CB-CG-CD	5.20	121.43	112.60
1	C	533	LYS	N-CA-C	-5.20	104.68	111.02
2	D	345	ILE	CA-CB-CG1	-5.20	101.57	110.40
1	A	600	ILE	N-CA-C	5.19	116.20	108.46
2	B	394	ARG	N-CA-C	5.19	119.48	113.20
1	C	666	PRO	N-CA-CB	5.19	109.00	103.39
2	D	318	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	522	PRO	N-CA-CB	5.19	107.94	103.27
2	B	90	VAL	CA-C-N	5.19	127.61	120.39
2	B	90	VAL	C-N-CA	5.19	127.61	120.39
2	D	551	ALA	CA-C-O	-5.19	115.36	121.07
2	B	427	GLY	N-CA-C	5.19	123.36	115.63
2	D	98	THR	N-CA-CB	-5.19	101.31	109.51
2	D	127	GLU	CA-CB-CG	-5.19	103.72	114.10
2	B	163	LYS	CA-C-N	5.19	129.94	123.14
2	B	163	LYS	C-N-CA	5.19	129.94	123.14
1	C	131	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	C	178	TYR	CA-C-N	5.19	127.10	120.56
1	C	178	TYR	C-N-CA	5.19	127.10	120.56
1	C	515	ILE	CA-C-N	5.19	127.19	120.44
1	C	515	ILE	C-N-CA	5.19	127.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	CA-CB-CG	5.19	124.48	114.10
2	D	66	THR	CA-C-N	5.19	127.29	120.60
2	D	66	THR	C-N-CA	5.19	127.29	120.60
1	C	72	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	C	86	ILE	CA-C-N	-5.19	115.24	123.23
1	C	86	ILE	C-N-CA	-5.19	115.24	123.23
2	B	212	PRO	N-CA-CB	5.18	107.94	103.27
1	C	584	ARG	NE-CZ-NH2	5.18	123.87	119.20
2	B	217	LEU	O-C-N	-5.18	116.53	122.08
2	B	463	VAL	CA-C-O	-5.18	114.30	120.78
2	B	499	GLN	N-CA-C	-5.18	105.32	110.97
1	C	361	GLN	CA-CB-CG	5.18	124.47	114.10
2	D	149	HIS	CA-CB-CG	5.18	118.98	113.80
2	D	362	PRO	N-CA-CB	5.18	108.15	103.33
1	A	53	ASP	CA-C-N	5.18	129.51	120.86
1	A	53	ASP	C-N-CA	5.18	129.51	120.86
1	A	592	GLN	N-CA-CB	5.18	117.73	110.12
2	B	452	ARG	CA-C-O	-5.18	114.93	120.42
2	D	243	ASN	N-CA-C	5.18	121.83	110.80
2	D	448	GLU	O-C-N	-5.17	116.64	122.12
1	A	386	THR	CA-C-N	5.17	127.64	120.29
1	A	386	THR	C-N-CA	5.17	127.64	120.29
2	B	602	PHE	CB-CA-C	-5.17	100.23	110.27
2	D	356	GLU	CB-CA-C	5.17	120.93	110.38
2	D	495	GLU	CA-CB-CG	-5.17	103.76	114.10
2	D	570	SER	CA-C-O	-5.17	115.99	121.94
2	B	39	VAL	CA-C-O	-5.17	115.37	120.85
2	B	342	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	D	272	THR	N-CA-CB	5.17	117.51	110.38
2	D	470	GLY	CA-C-O	-5.17	113.22	119.68
1	A	580	VAL	O-C-N	-5.17	116.51	121.83
2	B	310	VAL	O-C-N	-5.17	116.86	121.87
1	C	9	SER	N-CA-CB	-5.17	104.03	110.90
1	C	192	LEU	N-CA-C	5.17	117.15	109.25
1	C	193	ALA	CA-C-O	5.17	126.00	120.32
1	A	642	ARG	CG-CD-NE	5.16	123.36	112.00
2	B	489	ALA	CB-CA-C	5.16	118.96	109.46
1	C	562	GLN	CB-CG-CD	5.16	121.38	112.60
2	D	599	PHE	N-CA-C	-5.16	105.55	111.07
1	A	202	LYS	N-CA-C	-5.16	105.83	111.82
2	B	328	TRP	N-CA-C	-5.16	105.10	111.40
2	B	552	GLU	CB-CG-CD	-5.16	103.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	419	LYS	O-C-N	-5.16	116.72	122.09
2	D	253	ALA	CA-C-N	5.16	127.71	120.28
2	D	253	ALA	C-N-CA	5.16	127.71	120.28
1	C	173	PRO	CB-CA-C	-5.16	104.11	112.62
1	C	237	SER	CA-C-N	5.16	127.89	122.11
1	C	237	SER	C-N-CA	5.16	127.89	122.11
1	A	339	GLN	CG-CD-NE2	5.16	124.14	116.40
1	A	379	SER	CA-CB-OG	5.16	121.41	111.10
1	C	189	PRO	CA-C-N	5.16	131.39	121.18
1	C	189	PRO	C-N-CA	5.16	131.39	121.18
1	C	207	ARG	CA-C-N	5.16	129.44	122.07
1	C	207	ARG	C-N-CA	5.16	129.44	122.07
1	A	131	ARG	CG-CD-NE	5.15	123.34	112.00
1	A	468	ASN	CA-CB-CG	5.15	117.75	112.60
1	C	685	GLY	CA-C-O	5.15	127.10	121.48
2	B	92	PRO	CA-C-N	5.15	132.92	124.31
2	B	92	PRO	C-N-CA	5.15	132.92	124.31
1	C	161	MET	CB-CA-C	-5.15	100.43	109.71
1	C	289	GLY	O-C-N	-5.15	117.03	123.21
1	C	191	GLN	CG-CD-NE2	5.15	124.13	116.40
2	D	126	LEU	CA-C-N	5.15	127.49	120.54
2	D	126	LEU	C-N-CA	5.15	127.49	120.54
1	C	175	LEU	CA-C-N	5.15	127.13	120.44
1	C	175	LEU	C-N-CA	5.15	127.13	120.44
2	D	351	SER	CA-C-N	5.15	127.52	120.46
2	D	351	SER	C-N-CA	5.15	127.52	120.46
1	A	696	LEU	CA-C-N	5.15	127.13	120.44
1	A	696	LEU	C-N-CA	5.15	127.13	120.44
2	D	88	PRO	O-C-N	-5.15	116.48	122.86
1	A	127	SER	N-CA-C	5.14	119.03	112.34
1	A	291	GLY	CA-C-N	5.14	128.13	120.31
1	A	291	GLY	C-N-CA	5.14	128.13	120.31
1	A	401	ASP	CA-CB-CG	5.14	117.75	112.60
1	C	468	ASN	CA-C-N	5.14	131.00	121.94
1	C	468	ASN	C-N-CA	5.14	131.00	121.94
1	C	694	ASP	CB-CG-OD1	5.14	130.23	118.40
2	D	169	ARG	CB-CA-C	5.14	118.60	109.75
2	D	397	ASP	O-C-N	-5.14	115.40	121.32
1	A	617	ILE	CA-C-O	-5.14	115.92	121.27
2	B	341	LEU	CA-C-N	5.14	127.12	120.44
2	B	341	LEU	C-N-CA	5.14	127.12	120.44
1	C	695	GLU	CA-C-O	-5.14	115.42	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	510	ARG	CA-C-N	5.14	125.08	119.78
2	D	510	ARG	C-N-CA	5.14	125.08	119.78
1	A	105	ASN	N-CA-CB	5.14	117.68	110.12
1	A	131	ARG	NE-CZ-NH1	5.14	126.64	121.50
2	B	576	GLN	CA-C-N	-5.14	114.58	122.60
2	B	576	GLN	C-N-CA	-5.14	114.58	122.60
2	D	168	SER	N-CA-CB	-5.14	103.07	111.66
2	D	340	ILE	CB-CG1-CD1	5.14	124.59	113.80
1	A	553	GLU	O-C-N	-5.14	115.95	122.27
1	C	97	GLU	CA-C-N	5.14	127.48	120.54
1	C	97	GLU	C-N-CA	5.14	127.48	120.54
1	C	514	LYS	CA-CB-CG	-5.14	103.83	114.10
2	D	78	PRO	O-C-N	-5.14	116.63	122.18
1	C	514	LYS	O-C-N	-5.13	116.78	122.07
1	C	532	LEU	N-CA-C	-5.13	105.60	111.14
2	B	582	ALA	N-CA-C	-5.13	105.38	110.97
2	D	74	PRO	N-CA-CB	5.13	108.96	103.52
2	D	223	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	C	17	VAL	N-CA-C	-5.13	102.47	107.55
2	D	292	LEU	CA-C-N	5.13	127.15	120.28
2	D	292	LEU	C-N-CA	5.13	127.15	120.28
2	B	237	ASP	CA-C-O	-5.12	115.45	120.98
2	D	492	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	20	ASP	CB-CG-OD1	5.12	130.18	118.40
1	A	662	LEU	O-C-N	5.12	128.21	122.22
1	C	525	LYS	CA-C-N	5.12	129.04	122.64
1	C	525	LYS	C-N-CA	5.12	129.04	122.64
1	A	272	SER	O-C-N	-5.12	116.23	122.22
1	A	512	LEU	CB-CA-C	5.12	118.84	110.96
2	B	152	GLU	O-C-N	-5.12	116.32	122.15
1	A	281	ALA	N-CA-CB	5.12	117.92	110.30
1	A	521	ASN	O-C-N	-5.11	116.77	121.42
2	B	149	HIS	CA-C-N	5.11	129.32	121.19
2	B	149	HIS	C-N-CA	5.11	129.32	121.19
2	B	336	PRO	O-C-N	-5.11	115.62	122.22
2	B	458	GLN	N-CA-C	-5.11	97.98	108.21
1	C	564	ARG	CA-CB-CG	5.11	124.33	114.10
2	D	401	GLY	O-C-N	-5.11	117.33	122.65
2	D	527	ARG	CA-C-O	-5.11	115.13	120.55
2	B	533	PRO	N-CA-CB	5.11	108.70	103.23
1	A	203	GLU	N-CA-C	-5.11	105.60	111.07
2	B	502	ASP	CA-C-N	5.11	127.89	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	ASP	C-N-CA	5.11	127.89	120.79
1	C	335	SER	O-C-N	-5.11	115.75	122.39
2	D	312	GLY	N-CA-C	5.11	120.94	113.48
2	B	524	PHE	N-CA-C	5.10	119.51	113.28
1	C	429	LYS	N-CA-C	-5.10	105.80	111.36
1	A	686	GLY	O-C-N	-5.10	116.37	123.56
1	A	708	GLY	CA-C-N	5.10	128.35	121.05
1	A	708	GLY	C-N-CA	5.10	128.35	121.05
2	B	130	GLU	CB-CG-CD	5.10	121.27	112.60
1	C	74	PRO	CB-CA-C	-5.10	104.89	112.55
1	C	204	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	491	GLU	CA-C-N	5.10	128.06	120.31
1	A	491	GLU	C-N-CA	5.10	128.06	120.31
1	C	244	ALA	O-C-N	-5.10	115.77	122.39
1	C	537	ASP	O-C-N	-5.10	116.34	122.15
2	D	365	GLN	CB-CG-CD	5.10	121.26	112.60
2	D	562	ALA	O-C-N	5.09	128.66	122.85
1	A	577	THR	CA-C-N	5.09	124.70	119.05
1	A	577	THR	C-N-CA	5.09	124.70	119.05
2	B	142	PRO	N-CA-CB	5.09	108.93	103.33
2	B	343	GLY	O-C-N	-5.09	117.29	122.18
1	C	55	TYR	CA-C-N	5.09	131.26	121.54
1	C	55	TYR	C-N-CA	5.09	131.26	121.54
1	A	363	LEU	CA-C-O	5.09	126.69	120.99
2	B	264	ARG	CA-C-N	5.09	127.41	120.54
2	B	264	ARG	C-N-CA	5.09	127.41	120.54
2	B	560	SER	CB-CA-C	-5.09	102.03	110.68
2	D	93	PHE	N-CA-CB	-5.09	105.92	114.27
2	D	517	CYS	N-CA-CB	-5.09	102.06	109.95
2	D	621	MET	CA-C-N	-5.09	115.43	122.30
2	D	621	MET	C-N-CA	-5.09	115.43	122.30
1	A	533	LYS	N-CA-C	-5.09	105.42	110.97
1	A	636	THR	CA-C-N	5.09	124.70	119.05
1	A	636	THR	C-N-CA	5.09	124.70	119.05
1	C	689	PRO	N-CA-CB	5.09	107.84	103.31
2	D	176	ALA	O-C-N	-5.09	116.26	122.11
1	A	228	THR	N-CA-CB	5.08	117.38	110.01
2	B	328	TRP	N-CA-CB	5.08	117.65	110.13
1	C	447	GLU	O-C-N	-5.08	116.36	122.15
1	C	536	ILE	O-C-N	-5.08	116.93	121.91
1	C	560	THR	CA-C-O	-5.08	114.82	120.66
2	D	22	SER	N-CA-CB	-5.08	101.78	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	MET	N-CA-C	5.08	116.03	108.31
1	C	104	ARG	CA-C-N	5.08	127.40	120.54
1	C	104	ARG	C-N-CA	5.08	127.40	120.54
1	A	540	ARG	CA-CB-CG	-5.08	103.94	114.10
2	B	117	ASP	CA-C-O	5.08	126.54	120.70
2	B	304	TRP	CA-C-N	5.08	127.09	120.28
2	B	304	TRP	C-N-CA	5.08	127.09	120.28
2	B	493	ASP	N-CA-CB	5.08	117.59	110.12
2	D	73	VAL	O-C-N	-5.08	115.31	121.10
2	D	622	ASP	N-CA-C	-5.08	100.89	108.96
1	A	284	LEU	N-CA-C	-5.08	102.18	110.20
1	A	341	VAL	CA-C-N	5.08	129.20	120.72
1	A	341	VAL	C-N-CA	5.08	129.20	120.72
2	B	457	LYS	O-C-N	-5.08	115.46	122.46
1	C	515	ILE	N-CA-CB	5.08	116.49	110.55
1	C	582	GLU	CG-CD-OE2	5.08	130.08	118.40
1	A	41	ALA	N-CA-CB	5.07	118.03	110.22
1	A	211	ILE	CA-C-O	5.07	127.12	120.78
1	C	357	GLN	CA-C-N	5.07	131.36	121.41
1	C	357	GLN	C-N-CA	5.07	131.36	121.41
1	C	426	GLU	O-C-N	-5.07	116.65	122.08
2	B	421	GLN	O-C-N	-5.07	116.75	122.03
1	C	380	ALA	CA-C-O	-5.07	114.14	119.97
2	B	527	ARG	O-C-N	-5.07	116.75	122.12
2	B	564	VAL	CG1-CB-CG2	-5.07	99.65	110.80
2	B	574	TYR	O-C-N	-5.07	116.75	122.12
1	C	670	LYS	CA-C-O	-5.07	115.47	120.90
2	D	463	VAL	CA-C-N	-5.07	114.20	122.26
2	D	463	VAL	C-N-CA	-5.07	114.20	122.26
1	A	599	ARG	CA-CB-CG	5.07	124.24	114.10
2	B	94	THR	CA-C-N	5.07	129.18	120.72
2	B	94	THR	C-N-CA	5.07	129.18	120.72
2	B	593	LEU	N-CA-CB	-5.07	102.30	110.81
2	D	435	THR	OG1-CB-CG2	-5.07	99.17	109.30
2	D	555	GLU	CA-C-O	-5.07	115.50	120.82
1	A	558	ARG	CA-C-N	-5.07	112.98	121.39
1	A	558	ARG	C-N-CA	-5.07	112.98	121.39
2	B	425	LYS	CA-C-N	5.06	132.07	121.94
2	B	425	LYS	C-N-CA	5.06	132.07	121.94
1	A	328	HIS	N-CA-CB	5.06	118.46	110.56
2	B	66	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	330	GLN	CA-C-O	5.06	125.94	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	LEU	O-C-N	-5.06	117.61	123.33
2	D	628	SER	CA-C-O	5.06	126.63	121.07
1	C	60	TRP	CA-C-N	5.05	127.56	120.28
1	C	60	TRP	C-N-CA	5.05	127.56	120.28
1	C	387	GLN	OE1-CD-NE2	5.05	127.66	122.60
2	B	263	VAL	CA-C-O	-5.05	115.44	121.05
2	B	511	PRO	CA-C-O	-5.05	115.70	121.56
1	C	123	ARG	NE-CZ-NH2	-5.05	114.65	119.20
2	D	42	VAL	CB-CA-C	-5.05	105.50	111.97
2	B	224	LEU	O-C-N	-5.05	115.40	122.37
2	B	387	ALA	N-CA-C	5.05	116.86	111.36
1	C	692	ASP	CA-C-O	-5.05	112.65	119.11
1	C	150	ARG	CG-CD-NE	-5.05	100.89	112.00
1	A	79	TYR	N-CA-C	5.05	119.28	113.18
1	C	322	SER	CA-C-N	5.05	132.03	121.94
1	C	322	SER	C-N-CA	5.05	132.03	121.94
1	C	595	GLY	CA-C-N	5.05	131.47	122.09
1	C	595	GLY	C-N-CA	5.05	131.47	122.09
2	D	473	SER	CA-C-N	5.05	129.67	121.95
2	D	473	SER	C-N-CA	5.05	129.67	121.95
2	B	339	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	A	351	GLU	CA-C-O	-5.04	115.52	120.82
1	C	5	PRO	CA-C-O	5.04	127.08	121.43
2	D	409	THR	N-CA-C	-5.04	105.69	111.14
1	A	268	ARG	NH1-CZ-NH2	5.04	125.85	119.30
2	B	75	MET	N-CA-C	5.04	117.28	108.76
2	B	523	ASP	CB-CA-C	-5.04	101.33	110.56
1	C	174	ILE	CA-C-O	5.04	126.19	120.85
1	C	645	VAL	CB-CA-C	5.04	118.42	111.97
2	D	169	ARG	CG-CD-NE	5.04	123.09	112.00
1	A	719	VAL	O-C-N	-5.04	116.52	121.96
1	C	498	LYS	CA-C-O	-5.04	115.51	120.90
1	A	578	PRO	N-CA-CB	5.04	108.87	103.33
1	A	595	GLY	O-C-N	-5.04	116.04	122.43
1	A	712	PRO	N-CA-C	-5.04	106.27	113.47
1	C	326	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	112	GLY	N-CA-C	-5.03	103.18	111.38
1	C	241	SER	CA-CB-OG	5.03	121.17	111.10
2	D	27	PHE	O-C-N	5.03	125.63	121.35
2	D	42	VAL	N-CA-C	5.03	115.25	110.42
1	C	647	ALA	O-C-N	-5.03	116.16	122.35
2	D	468	MET	O-C-N	5.03	129.88	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	TYR	CB-CA-C	-5.03	100.34	109.45
2	D	59	LEU	O-C-N	-5.03	116.79	122.12
1	C	588	GLU	N-CA-C	-5.03	105.69	111.07
1	A	530	ASN	CB-CG-ND2	-5.03	108.86	116.40
2	B	185	ARG	CA-C-O	-5.03	113.32	120.51
2	B	254	TRP	N-CA-CB	5.03	117.96	110.22
2	B	457	LYS	CA-CB-CG	5.03	124.15	114.10
2	D	217	LEU	N-CA-CB	5.03	118.98	110.49
2	D	292	LEU	O-C-N	-5.03	116.66	122.09
2	B	403	TYR	CB-CG-CD2	-5.02	113.27	120.80
2	B	410	ARG	NE-CZ-NH2	-5.02	114.68	119.20
2	D	226	LYS	N-CA-C	-5.02	104.89	111.02
2	D	518	LEU	CA-C-O	5.02	126.84	121.16
1	C	405	GLY	O-C-N	-5.02	117.43	122.65
1	C	476	PRO	N-CA-CB	5.02	107.95	103.08
1	A	454	GLN	O-C-N	-5.02	116.87	122.09
2	B	291	PHE	CA-CB-CG	5.02	118.82	113.80
1	C	599	ARG	O-C-N	5.02	129.18	123.31
1	C	720	LYS	N-CA-CB	-5.02	102.74	110.12
1	A	96	LYS	CA-C-N	5.02	127.26	120.44
1	A	96	LYS	C-N-CA	5.02	127.26	120.44
1	A	572	LYS	N-CA-CB	5.02	117.42	109.94
1	C	225	PHE	CA-CB-CG	5.02	118.82	113.80
2	D	466	PHE	O-C-N	-5.02	119.22	121.53
2	D	555	GLU	CB-CG-CD	5.02	121.13	112.60
1	C	203	GLU	N-CA-C	-5.02	105.72	111.14
1	C	475	GLU	CB-CA-C	-5.02	102.16	109.38
1	A	188	LYS	O-C-N	-5.01	115.27	121.64
2	B	626	THR	O-C-N	-5.01	116.81	122.12
1	A	102	TYR	O-C-N	-5.01	116.81	122.12
1	A	318	LYS	N-CA-C	-5.01	107.55	113.97
2	B	429	MET	CA-C-N	5.01	127.25	120.38
2	B	429	MET	C-N-CA	5.01	127.25	120.38
2	D	264	ARG	CB-CG-CD	5.01	122.82	111.30
1	A	443	LYS	CA-C-N	5.01	127.40	120.29
1	A	443	LYS	C-N-CA	5.01	127.40	120.29
1	C	283	ARG	CD-NE-CZ	5.01	131.41	124.40
2	D	243	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	309	ALA	CA-C-N	5.01	127.25	120.44
1	A	309	ALA	C-N-CA	5.01	127.25	120.44
1	C	582	GLU	O-C-N	-5.01	116.91	122.07
2	D	374	PHE	CB-CA-C	5.00	120.03	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	THR	CB-CA-C	-5.00	100.56	109.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	GLY	Mainchain
2	B	401	GLY	Mainchain
1	C	593	ALA	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5558	0	5441	72	0
1	C	5558	0	5440	75	0
2	B	4695	0	4610	44	0
2	D	4695	0	4610	83	0
3	A	91	0	88	16	0
3	C	91	0	88	16	0
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	454	0	0	3	0
5	B	316	0	0	1	0
5	C	490	0	0	4	0
5	D	265	0	0	0	0
All	All	22307	0	20341	283	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 7.

All (283) 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:C:800:B12:H363	3:C:800:B12:H421	1.27	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:800:B12:H421	3:C:800:B12:C36	1.80	1.11
3:C:800:B12:H552	3:C:800:B12:H531	1.26	1.10
3:A:800:B12:H363	3:A:800:B12:H421	1.07	1.05
3:A:800:B12:H421	3:A:800:B12:C36	1.90	1.01
3:A:800:B12:H363	3:A:800:B12:C42	1.96	0.95
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.17	0.92
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.25	0.85
3:C:800:B12:C36	3:C:800:B12:C42	2.54	0.84
1:C:374:LEU:HB2	1:C:481:LEU:HD23	1.67	0.77
3:A:800:B12:H531	3:A:800:B12:H552	1.67	0.77
1:A:188:LYS:H	1:A:191:GLN:NE2	1.83	0.77
2:D:468:MET:HE3	2:D:471:ALA:HA	1.66	0.75
1:C:188:LYS:H	1:C:191:GLN:NE2	1.85	0.75
1:C:247:GLU:HB3	3:C:800:B12:H532	1.68	0.75
1:A:374:LEU:HB2	1:A:481:LEU:HD23	1.69	0.74
1:C:503:ARG:HD2	1:C:508:VAL:HG21	1.70	0.74
3:C:800:B12:H531	3:C:800:B12:C55	2.11	0.73
1:C:357:GLN:HE22	2:D:290:GLN:NE2	1.86	0.73
1:C:188:LYS:H	1:C:191:GLN:HE21	1.37	0.72
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.70	0.72
2:D:202:ILE:HD12	2:D:258:THR:HG23	1.71	0.72
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.72	0.72
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.70	0.72
2:D:297:LEU:HD12	2:D:353:GLY:HA3	1.72	0.71
1:A:133:ALA:HB1	1:A:489:LEU:HD21	1.72	0.71
1:A:650:HIS:HB3	1:A:722:LEU:HD21	1.73	0.70
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.74	0.69
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.73	0.69
2:D:284:VAL:HG11	2:D:322:GLN:HE21	1.57	0.68
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.75	0.68
1:C:112:GLY:HA2	1:C:161:MET:HE1	1.74	0.67
1:A:357:GLN:HE22	2:B:290:GLN:NE2	1.92	0.67
1:C:652:VAL:HG11	1:C:668:LEU:HD11	1.78	0.65
2:B:246:ALA:HB1	2:B:250:ALA:HB3	1.79	0.65
3:C:800:B12:H302	3:C:800:B12:H353	1.77	0.65
1:A:94:THR:HG22	1:A:488:VAL:HG13	1.78	0.65
3:C:800:B12:H351	3:C:800:B12:H372	1.79	0.64
3:C:800:B12:H363	3:C:800:B12:C42	2.16	0.64
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.78	0.64
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.80	0.63
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.81	0.63
2:D:121:THR:HG21	2:D:145:ILE:HD11	1.81	0.62
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.79	0.62
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.80	0.62
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.45	0.62
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.82	0.61
2:D:391:ASN:HB3	2:D:394:ARG:HD2	1.81	0.61
1:A:683:THR:HG22	1:A:703:GLU:HB2	1.81	0.61
1:C:317:PRO:HG2	1:C:323:MET:HE2	1.83	0.60
3:C:800:B12:H421	3:C:800:B12:H361	1.77	0.60
2:D:292:LEU:HD23	2:D:408:LEU:HD21	1.82	0.60
2:D:82:PRO:HD2	2:D:406:GLU:HG3	1.83	0.60
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.84	0.60
1:A:188:LYS:H	1:A:191:GLN:HE21	1.50	0.60
1:A:161:MET:HE3	1:A:162:SER:H	1.67	0.59
1:A:247:GLU:HB3	3:A:800:B12:H532	1.84	0.59
1:C:638:GLU:HA	1:C:671:GLU:HG3	1.83	0.59
3:A:800:B12:H2B	3:A:800:B12:O7R	2.00	0.59
1:C:139:ALA:HB1	3:C:800:B12:H362	1.85	0.59
1:A:684:VAL:HG12	1:A:688:ILE:HD11	1.84	0.59
2:B:220:TRP:HA	2:B:220:TRP:CE3	2.38	0.59
2:D:297:LEU:HA	2:D:322:GLN:HE22	1.67	0.58
3:A:800:B12:H351	3:A:800:B12:H372	1.85	0.58
2:D:402:SER:HB3	2:D:405:VAL:HB	1.85	0.58
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.84	0.58
3:A:800:B12:H531	3:A:800:B12:C55	2.35	0.57
1:A:617:ILE:HD13	1:A:711:ILE:HG12	1.86	0.57
1:C:24:ARG:HH22	2:D:315:GLU:HG3	1.69	0.57
1:C:392:GLN:HB3	2:D:459:PRO:HG2	1.87	0.57
1:A:599:ARG:HG2	1:A:649:VAL:HA	1.86	0.57
1:A:359:HIS:HE1	1:A:401:ASP:H	1.52	0.57
1:C:359:HIS:HE1	1:C:401:ASP:H	1.51	0.57
2:D:179:LEU:HG	2:D:195:LEU:HD12	1.87	0.56
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.51	0.56
2:B:552:GLU:HA	2:B:555:GLU:HG2	1.87	0.56
2:D:100:ARG:HD2	2:D:396:ASN:HA	1.87	0.56
2:D:80:ASP:HB3	2:D:407:SER:HB2	1.87	0.56
1:A:359:HIS:CE1	1:A:401:ASP:H	2.24	0.56
2:D:220:TRP:HA	2:D:220:TRP:CE3	2.40	0.55
1:C:372:ILE:HD13	1:C:478:LEU:HD23	1.87	0.55
2:D:27:PHE:HB3	2:D:28:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:HIS:CE1	1:C:401:ASP:H	2.24	0.55
1:A:579:GLU:HB3	1:A:712:PRO:HB2	1.89	0.55
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.37	0.55
2:D:281:ASN:ND2	2:D:323:ASN:HD21	2.04	0.55
2:D:423:VAL:HG13	2:D:432:ALA:HB2	1.89	0.54
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.88	0.54
2:D:141:ASP:HB3	2:D:142:PRO:HD2	1.89	0.54
2:D:617:LEU:HD22	2:D:621:MET:HE1	1.88	0.54
2:D:284:VAL:HG21	2:D:297:LEU:HD22	1.89	0.54
1:C:65:ALA:HB2	1:C:72:HIS:HB2	1.90	0.53
2:D:91:ALA:HA	2:D:92:PRO:C	2.32	0.53
3:A:800:B12:O7R	3:A:800:B12:C2B	2.56	0.53
1:A:21:ALA:HA	2:B:90:VAL:HG11	1.90	0.53
3:C:800:B12:C42	3:C:800:B12:H361	2.35	0.53
2:D:238:ALA:HB1	2:D:251:GLU:HG3	1.91	0.53
1:A:599:ARG:HH21	1:A:647:ALA:HB1	1.74	0.53
1:A:311:LEU:HD11	1:A:424:ILE:HD13	1.91	0.52
1:C:448:GLU:HG2	1:C:569:VAL:HG21	1.90	0.52
1:A:710:VAL:HG12	1:A:712:PRO:HD2	1.90	0.52
1:C:599:ARG:HG3	1:C:649:VAL:HA	1.92	0.52
1:A:24:ARG:HH22	2:B:315:GLU:HG3	1.73	0.52
1:C:386:THR:HA	2:D:341:LEU:HD13	1.92	0.52
2:D:305:ALA:HA	2:D:318:ARG:HB3	1.90	0.51
2:D:92:PRO:O	2:D:93:PHE:HB2	2.10	0.51
2:D:146:ALA:HB3	2:D:149:HIS:ND1	2.26	0.51
2:D:331:LEU:HD11	2:D:361:LEU:HD12	1.93	0.51
1:A:706:THR:HB	1:A:707:PRO:CD	2.41	0.51
1:A:139:ALA:HB1	3:A:800:B12:H362	1.93	0.51
1:C:20:ASP:OD2	1:C:24:ARG:HD2	2.11	0.51
1:A:498:LYS:HG3	1:C:23:ARG:NH2	2.26	0.51
2:D:158:LEU:HD12	2:D:161:MET:SD	2.51	0.50
2:D:598:ALA:HB3	2:D:601:GLU:HG3	1.93	0.50
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.91	0.50
2:D:91:ALA:HB1	2:D:92:PRO:HA	1.94	0.49
2:D:166:VAL:HG22	2:D:179:LEU:HD22	1.94	0.49
2:D:370:PRO:HB3	2:D:375:PRO:HG2	1.93	0.49
2:D:331:LEU:HD13	2:D:365:GLN:HB3	1.94	0.49
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.95	0.49
3:C:800:B12:H552	3:C:800:B12:C53	2.16	0.49
1:A:215:GLN:HB3	1:A:216:PRO:CD	2.42	0.49
1:C:390:LEU:HA	1:C:394:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:THR:HB	1:C:707:PRO:CD	2.43	0.49
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.59	0.49
1:A:4:LEU:N	1:A:5:PRO:HD3	2.27	0.49
1:A:201:LEU:HG	1:A:218:MET:HE1	1.93	0.48
3:C:800:B12:O5	3:C:800:B12:O7R	2.26	0.48
1:A:8:ASP:HB2	2:B:425:LYS:HE2	1.94	0.48
2:D:129:LEU:HD11	2:D:136:LEU:HD21	1.94	0.48
2:D:264:ARG:HG3	2:D:311:PHE:HZ	1.79	0.48
1:A:123:ARG:HD3	1:A:607:GLN:OE1	2.14	0.48
1:C:8:ASP:HB2	2:D:425:LYS:HE2	1.94	0.48
1:A:310:LYS:HE2	2:B:21:LEU:HD11	1.95	0.48
3:A:800:B12:H492	3:A:800:B12:C47	2.43	0.48
3:A:800:B12:H551	3:A:800:B12:C61	2.44	0.48
1:A:586:LEU:HB3	1:A:719:VAL:HG11	1.96	0.47
2:B:152:GLU:O	2:B:155:SER:HB2	2.13	0.47
2:B:391:ASN:ND2	2:B:394:ARG:HE	2.11	0.47
1:C:512:LEU:HD21	1:C:543:ALA:HB1	1.96	0.47
1:C:122:HIS:HA	1:C:167:MET:HE1	1.95	0.47
1:A:112:GLY:HA2	1:A:161:MET:HE1	1.96	0.47
2:D:143:ASP:HA	2:D:480:PRO:HB2	1.95	0.47
1:A:5:PRO:HD2	2:B:311:PHE:CE1	2.49	0.47
1:A:358:GLY:O	1:A:359:HIS:HB2	2.14	0.47
1:C:203:GLU:OE1	1:C:207:ARG:HB3	2.15	0.47
1:A:511:ALA:HB1	1:A:538:ALA:HA	1.96	0.47
2:D:125:ILE:HG23	2:D:136:LEU:HD11	1.96	0.47
2:B:364:THR:HA	2:B:367:LEU:HD12	1.96	0.47
1:C:369:ASP:HB3	1:C:478:LEU:HD21	1.96	0.47
1:A:613:GLY:HA2	3:A:800:B12:H3P1	1.97	0.47
2:D:260:ALA:O	2:D:261:GLU:C	2.58	0.46
2:B:252:LEU:HD11	2:B:300:LEU:HA	1.96	0.46
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.97	0.46
2:D:133:VAL:HG23	2:D:380:ARG:HD3	1.97	0.46
1:C:431:GLY:HA3	1:C:435:LYS:HD2	1.97	0.46
1:A:172:LEU:HD11	1:A:220:ILE:HG23	1.97	0.46
2:D:88:PRO:HG2	2:D:99:VAL:HG22	1.98	0.46
1:C:128:ASP:HB3	1:C:493:LYS:HG2	1.98	0.46
2:D:435:THR:HG22	2:D:436:GLU:H	1.81	0.46
2:D:637:ALA:O	2:D:638:LYS:HB3	2.15	0.46
2:B:435:THR:HG22	2:B:436:GLU:H	1.80	0.46
1:A:521:ASN:O	1:A:529:ARG:HD3	2.16	0.46
3:A:800:B12:H353	3:A:800:B12:H302	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ASN:O	1:C:15:ALA:C	2.59	0.45
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.98	0.45
1:C:599:ARG:CG	1:C:649:VAL:HA	2.46	0.45
1:A:636:THR:HB	1:A:637:PRO:HD2	1.98	0.45
1:C:283:ARG:HD3	1:C:283:ARG:HA	1.87	0.45
2:B:73:VAL:HB	2:B:74:PRO:CD	2.43	0.45
1:A:79:TYR:HA	1:A:82:ARG:O	2.17	0.45
1:C:358:GLY:O	1:C:359:HIS:HB2	2.15	0.45
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.52	0.45
2:B:402:SER:HB3	2:B:405:VAL:HB	1.99	0.45
1:C:68:PRO:HA	1:C:69:PRO:HA	1.78	0.45
1:A:167:MET:HE3	1:A:174:ILE:HG13	1.98	0.45
1:A:529:ARG:HA	1:A:534:LEU:HD11	1.97	0.45
2:B:86:GLY:HA3	5:B:2047:HOH:O	2.16	0.44
1:C:426:GLU:O	1:C:427:VAL:C	2.59	0.44
3:C:800:B12:HM51	3:C:800:B12:HM63	1.56	0.44
1:A:500:ARG:HD3	5:A:2340:HOH:O	2.16	0.44
2:B:263:VAL:O	2:B:267:VAL:HG23	2.17	0.44
1:C:44:ILE:HD13	1:C:415:ASP:HB3	1.99	0.44
1:A:515:ILE:HD11	1:A:538:ALA:HB2	1.99	0.44
1:A:706:THR:HB	1:A:707:PRO:HD2	1.98	0.44
2:B:80:ASP:HB3	2:B:407:SER:HB2	1.99	0.44
1:C:197:GLN:HG3	1:C:239:SER:HB3	2.00	0.44
1:A:636:THR:HB	1:A:637:PRO:CD	2.48	0.44
2:D:586:LYS:HD2	2:D:590:ALA:HB3	1.99	0.44
2:B:503:ARG:NE	2:B:638:LYS:HB3	2.33	0.44
1:A:503:ARG:HD2	1:A:508:VAL:HG21	2.00	0.44
2:D:190:ALA:O	2:D:227:PHE:HA	2.17	0.44
2:D:381:ASN:HA	2:D:384:ILE:HB	2.00	0.44
2:B:236:ILE:HG23	2:B:258:THR:HG21	2.00	0.44
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.53	0.44
1:C:591:GLU:HA	1:C:596:ARG:O	2.18	0.44
1:C:162:SER:HA	1:C:193:ALA:O	2.18	0.43
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.99	0.43
2:B:397:ASP:O	2:B:398:PRO:C	2.61	0.43
2:B:421:GLN:O	2:B:422:GLU:C	2.61	0.43
1:C:684:VAL:O	1:C:704:ILE:HA	2.19	0.43
2:D:510:ARG:HA	2:D:511:PRO:HD3	1.93	0.43
1:C:520:GLY:N	1:C:555:VAL:HG21	2.34	0.43
1:A:544:THR:O	1:A:548:MET:HG3	2.18	0.43
1:C:161:MET:HE3	1:C:162:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:800:B12:H492	3:A:800:B12:H473	2.00	0.43
5:C:2490:HOH:O	2:D:42:VAL:HG21	2.19	0.43
1:A:514:LYS:HD3	1:A:534:LEU:HD22	2.00	0.43
2:B:191:LYS:HD2	2:B:226:LYS:O	2.19	0.43
2:B:532:SER:CB	2:B:533:PRO:HD3	2.46	0.43
2:D:461:THR:O	2:D:462:ALA:HB3	2.19	0.43
1:A:69:PRO:HG3	2:B:24:ALA:HA	2.01	0.43
1:A:85:THR:HB	1:A:362:SER:HB3	2.01	0.43
2:D:242:HIS:HB2	2:D:251:GLU:OE1	2.17	0.43
3:A:800:B12:H473	5:A:2443:HOH:O	2.19	0.42
1:C:118:ASP:HB2	5:C:2125:HOH:O	2.18	0.42
1:A:205:MET:HG3	1:A:442:PRO:HB2	2.01	0.42
2:D:275:GLU:O	2:D:279:THR:HG22	2.19	0.42
2:D:518:LEU:HD21	2:D:581:VAL:HG11	2.00	0.42
1:C:389:PHE:HA	2:D:461:THR:OG1	2.19	0.42
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.48	0.42
1:A:336:LEU:HD21	5:A:2255:HOH:O	2.19	0.42
2:D:264:ARG:HG3	2:D:311:PHE:CZ	2.55	0.42
1:A:129:ASN:HB3	1:A:132:VAL:HG22	2.02	0.42
2:B:527:ARG:HB3	2:B:568:CYS:HB3	2.01	0.42
1:C:25:PHE:O	1:C:26:GLU:C	2.63	0.42
1:A:299:ALA:HB1	1:A:413:THR:HA	2.01	0.42
1:A:336:LEU:HD12	1:A:370:GLU:HB3	2.02	0.42
1:C:215:GLN:HB3	1:C:216:PRO:CD	2.50	0.42
3:C:800:B12:H361	3:C:800:B12:H412	1.87	0.42
2:D:182:VAL:HG23	2:D:185:ARG:HH21	1.84	0.42
1:C:641:ALA:O	1:C:642:ARG:C	2.63	0.42
1:A:68:PRO:HA	1:A:69:PRO:HA	1.72	0.41
1:C:570:TYR:HB3	1:C:623:ASP:OD2	2.20	0.41
1:C:635:GLN:OE1	1:C:643:GLN:NE2	2.53	0.41
2:D:152:GLU:O	2:D:155:SER:HB3	2.20	0.41
1:A:405:GLY:O	1:A:406:SER:C	2.62	0.41
1:A:638:GLU:HA	1:A:671:GLU:HG3	2.02	0.41
2:D:354:GLY:O	2:D:355:ALA:C	2.62	0.41
1:A:346:VAL:O	1:A:350:ILE:HG12	2.21	0.41
1:A:526:ASP:HA	1:A:527:PRO:HD2	1.93	0.41
1:C:15:ALA:HA	1:C:16:PRO:HD2	1.86	0.41
1:C:261:ALA:O	1:C:262:ASP:C	2.63	0.41
2:D:166:VAL:O	2:D:167:PHE:HB3	2.21	0.41
2:D:399:ALA:O	2:D:400:GLY:C	2.63	0.41
1:C:214:PRO:O	1:C:215:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:HG12	1:C:317:PRO:HG3	2.02	0.41
1:C:401:ASP:HA	1:C:402:PRO:HD2	1.83	0.41
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.50	0.41
1:C:511:ALA:HB1	1:C:538:ALA:HA	2.03	0.41
5:C:2253:HOH:O	2:D:377:ARG:HD2	2.20	0.41
2:B:59:LEU:O	2:B:60:LYS:C	2.61	0.41
1:C:566:ILE:HD12	1:C:569:VAL:HG21	2.03	0.41
2:D:234:VAL:HB	2:D:280:ILE:HG23	2.02	0.41
1:A:152:LEU:HD23	1:A:153:PHE:CE2	2.55	0.41
1:A:261:ALA:O	1:A:262:ASP:C	2.62	0.41
1:C:18:PRO:HB2	1:C:20:ASP:OD1	2.21	0.41
1:C:412:LEU:O	1:C:413:THR:C	2.62	0.41
1:C:596:ARG:HD3	5:C:2401:HOH:O	2.21	0.41
1:A:171:VAL:HG21	1:A:198:ASN:ND2	2.35	0.41
2:B:244:ALA:HB1	2:B:442:LEU:HD13	2.02	0.41
1:C:66:GLY:HA2	1:C:74:PRO:O	2.20	0.41
1:C:296:MET:HE2	1:C:296:MET:HB2	1.93	0.41
1:C:307:LEU:HD22	1:C:421:TRP:CE3	2.56	0.41
2:D:90:VAL:HG12	2:D:91:ALA:O	2.20	0.41
2:D:149:HIS:O	2:D:150:LEU:C	2.64	0.41
2:D:314:ASP:O	2:D:315:GLU:C	2.64	0.41
2:D:315:GLU:O	2:D:318:ARG:HG3	2.21	0.41
2:D:406:GLU:O	2:D:407:SER:C	2.62	0.41
2:D:517:CYS:HB3	2:D:524:PHE:CD1	2.56	0.41
1:A:54:VAL:O	1:A:58:MET:HE3	2.21	0.41
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.18	0.41
1:A:6:ARG:HD3	2:B:264:ARG:NH1	2.36	0.40
2:B:442:LEU:HD12	2:B:488:LEU:HD22	2.03	0.40
2:D:91:ALA:HA	2:D:93:PHE:N	2.36	0.40
2:D:263:VAL:O	2:D:267:VAL:HG23	2.20	0.40
2:B:220:TRP:HA	2:B:220:TRP:HE3	1.83	0.40
1:C:40:THR:O	1:C:41:ALA:C	2.63	0.40
1:C:372:ILE:CG2	1:C:480:VAL:HG11	2.51	0.40
2:B:577:GLN:O	2:B:581:VAL:HG23	2.20	0.40
1:A:414:TRP:CZ2	1:A:418:ARG:HD3	2.56	0.40
2:B:632:ASP:O	2:B:633:ILE:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/727 (100%)	671 (93%)	51 (7%)	3 (0%)	30	49
1	C	725/727 (100%)	652 (90%)	62 (9%)	11 (2%)	8	16
2	B	617/637 (97%)	566 (92%)	47 (8%)	4 (1%)	21	39
2	D	617/637 (97%)	554 (90%)	56 (9%)	7 (1%)	11	23
All	All	2684/2728 (98%)	2443 (91%)	216 (8%)	25 (1%)	14	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	LYS
2	B	578	GLY
1	C	3	THR
1	C	8	ASP
1	C	573	GLU
2	D	435	THR
1	A	214	PRO
2	B	269	GLN
2	D	80	ASP
1	A	359	HIS
1	C	70	PHE
2	D	227	PHE
2	B	435	THR
1	C	214	PRO
1	C	359	HIS
1	C	430	VAL
2	D	185	ARG
2	D	400	GLY
2	D	600	LYS
1	C	206	VAL
1	C	486	SER
2	B	603	GLY

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Mol	Chain	Res	Type
1	A	206	VAL
2	D	308	GLY
1	C	15	ALA

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	570/589 (97%)	542 (95%)	28 (5%)	22	44
1	C	570/589 (97%)	540 (95%)	30 (5%)	20	41
2	B	474/509 (93%)	456 (96%)	18 (4%)	29	54
2	D	474/509 (93%)	437 (92%)	37 (8%)	11	25
All	All	2088/2196 (95%)	1975 (95%)	113 (5%)	20	40

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	LEU
1	A	53	ASP
1	A	67	ILE
1	A	131	ARG
1	A	200	ILE
1	A	202	LYS
1	A	206	VAL
1	A	207	ARG
1	A	241	SER
1	A	361	GLN
1	A	362	SER
1	A	365	THR
1	A	430	VAL
1	A	441	ILE
1	A	444	MET
1	A	473	GLU
1	A	485	ASN

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Mol	Chain	Res	Type
1	A	486	SER
1	A	487	THR
1	A	488	VAL
1	A	489	LEU
1	A	533	LYS
1	A	576	ASN
1	A	585	GLU
1	A	597	ARG
1	A	668	LEU
1	A	727	ASP
2	B	22	SER
2	B	60	LYS
2	B	67	VAL
2	B	83	LYS
2	B	119	LYS
2	B	161	MET
2	B	180	VAL
2	B	186	SER
2	B	216	VAL
2	B	334	GLU
2	B	440	LYS
2	B	532	SER
2	B	544	GLN
2	B	552	GLU
2	B	586	LYS
2	B	614	ASP
2	B	616	ARG
2	B	617	LEU
1	C	23	ARG
1	C	26	GLU
1	C	53	ASP
1	C	69	PRO
1	C	70	PHE
1	C	131	ARG
1	C	159	ASP
1	C	162	SER
1	C	198	ASN
1	C	200	ILE
1	C	202	LYS
1	C	207	ARG
1	C	221	ILE
1	C	222	SER

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Mol	Chain	Res	Type
1	C	241	SER
1	C	272	SER
1	C	414	TRP
1	C	430	VAL
1	C	438	GLU
1	C	444	MET
1	C	473	GLU
1	C	482	LYS
1	C	487	THR
1	C	488	VAL
1	C	576	ASN
1	C	585	GLU
1	C	592	GLN
1	C	668	LEU
1	C	713	GLU
1	C	727	ASP
2	D	20	THR
2	D	26	ASP
2	D	60	LYS
2	D	83	LYS
2	D	85	LEU
2	D	99	VAL
2	D	104	MET
2	D	119	LYS
2	D	129	LEU
2	D	145	ILE
2	D	155	SER
2	D	166	VAL
2	D	180	VAL
2	D	188	LYS
2	D	216	VAL
2	D	217	LEU
2	D	222	ARG
2	D	223	ARG
2	D	224	LEU
2	D	234	VAL
2	D	235	THR
2	D	264	ARG
2	D	272	THR
2	D	334	GLU
2	D	367	LEU
2	D	380	ARG

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Mol	Chain	Res	Type
2	D	429	MET
2	D	440	LYS
2	D	475	GLU
2	D	515	LEU
2	D	518	LEU
2	D	522	ARG
2	D	532	SER
2	D	553	ILE
2	D	593	LEU
2	D	614	ASP
2	D	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	191	GLN
1	A	198	ASN
1	A	359	HIS
1	A	385	ASN
1	A	635	GLN
1	A	643	GLN
2	B	290	GLN
2	B	323	ASN
2	B	391	ASN
2	B	577	GLN
1	C	191	GLN
1	C	198	ASN
1	C	359	HIS
1	C	385	ASN
1	C	492	GLN
1	C	562	GLN
2	D	196	ASN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN
2	D	391	ASN
2	D	421	GLN
2	D	437	HIS
2	D	544	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DCA	C	801	-	44,49,49	0.78	0	64,74,74	1.49	9 (14%)
3	B12	C	800	5,1	93,101,101	1.09	6 (6%)	146,166,166	2.26	49 (33%)
3	B12	A	800	1	93,101,101	1.07	5 (5%)	146,166,166	2.38	49 (33%)
4	DCA	A	801	-	44,49,49	0.72	0	64,74,74	1.53	12 (18%)

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
4	DCA	C	801	-	-	2/47/63/63	0/3/3/3
3	B12	C	800	5,1	-	11/56/223/223	0/3/11/11
3	B12	A	800	1	-	12/56/223/223	0/3/11/11
4	DCA	A	801	-	-	3/47/63/63	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	C54-C17	3.93	1.61	1.54
3	C	800	B12	C2B-N1B	-3.16	1.31	1.37
3	A	800	B12	C54-C17	3.10	1.59	1.54
3	A	800	B12	C14-N23	3.04	1.39	1.35
3	A	800	B12	C2B-N1B	-2.50	1.33	1.37
3	C	800	B12	C14-N23	2.27	1.38	1.35
3	A	800	B12	C6B-C5B	2.26	1.46	1.40
3	C	800	B12	C48-C13	2.24	1.59	1.54
3	A	800	B12	C48-C13	2.24	1.59	1.54
3	C	800	B12	C6B-C5B	2.06	1.46	1.40
3	C	800	B12	O8R-C5R	2.01	1.50	1.42

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C9B-C8B-N1B	8.83	109.08	105.35
3	C	800	B12	C55-C17-C18	8.37	127.33	111.15
3	C	800	B12	C13-C14-N23	7.39	119.16	109.10
3	A	800	B12	C13-C14-C15	-6.85	113.84	124.32
3	A	800	B12	C13-C14-N23	6.66	118.17	109.10
3	C	800	B12	C16-C15-C14	-6.55	111.31	121.25
3	A	800	B12	C16-C15-C14	-6.16	111.90	121.25
4	A	801	DCA	CDP-CBP-CAP	-6.14	98.17	108.82
4	C	801	DCA	C2P-C3P-N4P	5.98	132.15	111.52
3	A	800	B12	C55-C17-C18	5.76	122.28	111.15
3	C	800	B12	C53-C15-C16	5.62	130.05	120.38
3	A	800	B12	C53-C15-C16	5.19	129.31	120.38
3	A	800	B12	C47-C12-C46	-5.09	100.75	109.35
3	C	800	B12	C17-C16-C15	-4.94	118.48	126.26
3	A	800	B12	C55-C17-C16	4.85	126.23	116.65
3	C	800	B12	O5-P-O3	4.82	125.81	106.78
3	C	800	B12	C15-C16-N24	4.62	129.07	122.42
3	C	800	B12	C26-C2-C1	-4.60	102.85	110.01
3	A	800	B12	C1-C19-N24	-4.39	101.30	106.24
3	A	800	B12	C1P-N59-C57	-4.35	113.22	122.69
3	C	800	B12	C54-C17-C16	-4.33	89.93	112.40
3	A	800	B12	C54-C17-C16	-4.26	90.28	112.40
3	A	800	B12	C54-C17-C18	-4.21	106.77	112.98
3	C	800	B12	C30-C3-C2	4.14	127.85	119.09
3	C	800	B12	C13-C14-C15	-4.11	118.03	124.32
3	A	800	B12	C8B-C9B-N3B	-4.00	105.55	109.97
3	A	800	B12	C8-C9-C10	-3.96	114.78	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C54-C17-C55	-3.95	102.74	109.25
3	A	800	B12	C25-C2-C1	3.87	119.62	113.78
3	A	800	B12	C4B-C9B-N3B	3.87	137.14	130.51
3	A	800	B12	C2-C1-C19	-3.86	112.50	118.60
3	C	800	B12	C54-C17-C18	-3.84	107.32	112.98
3	A	800	B12	C17-C16-C15	-3.78	120.31	126.26
3	A	800	B12	C26-C2-C1	-3.67	104.28	110.01
3	C	800	B12	C12-C11-N23	3.52	116.74	111.83
3	C	800	B12	C20-C1-N21	3.49	116.00	110.27
3	C	800	B12	C31-C30-C3	-3.46	104.73	114.73
4	A	801	DCA	O2B-C2B-C3B	3.44	120.94	111.17
3	C	800	B12	C8-C9-C10	-3.37	116.05	123.32
3	A	800	B12	C20-C1-C2	3.36	118.89	113.28
3	C	800	B12	C7-C6-N22	3.35	114.07	107.94
3	A	800	B12	C18-C19-N24	3.31	107.35	102.31
3	C	800	B12	C47-C12-C46	-3.28	103.81	109.35
3	C	800	B12	C5M-C5B-C6B	-3.18	114.21	120.74
3	A	800	B12	C12-C13-C14	-3.17	96.95	102.26
3	A	800	B12	C49-C50-N52	3.13	126.24	116.51
3	C	800	B12	C20-C1-C19	3.12	112.36	109.36
3	C	800	B12	C54-C17-C55	-3.11	104.12	109.25
4	A	801	DCA	O5P-C5P-N4P	-3.10	117.16	123.01
3	A	800	B12	C12-C11-N23	3.08	116.12	111.83
3	C	800	B12	O6R-C1R-N1B	-3.05	102.05	108.06
3	A	800	B12	C5M-C5B-C6B	-3.03	114.53	120.74
3	C	800	B12	C41-C8-C9	-3.02	105.86	111.19
3	C	800	B12	C6-C5-C4	-3.00	116.16	121.54
3	A	800	B12	C41-C42-C43	2.97	122.65	112.59
3	A	800	B12	C4B-C9B-C8B	-2.96	117.30	120.15
3	C	800	B12	C12-C13-C14	-2.90	97.41	102.26
3	A	800	B12	C7B-C8B-N1B	-2.88	125.60	131.41
4	A	801	DCA	C2P-C3P-N4P	2.84	121.33	111.52
3	C	800	B12	C15-C14-N23	-2.84	122.79	126.26
3	A	800	B12	C8-C9-N22	2.83	116.41	110.77
3	C	800	B12	C6M-C6B-C7B	2.82	124.70	119.49
4	C	801	DCA	CDP-CBP-CCP	2.81	112.82	108.23
3	C	800	B12	C2-C1-C19	-2.81	114.17	118.60
3	C	800	B12	C35-C5-C4	2.76	122.42	116.79
3	A	800	B12	C6M-C6B-C5B	2.74	126.34	120.74
3	A	800	B12	C42-C41-C8	-2.72	106.88	114.73
3	C	800	B12	C48-C13-C12	-2.72	109.02	116.63
3	A	800	B12	C10-C9-N22	2.68	128.81	125.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	O63-C61-C60	2.68	126.51	120.87
3	C	800	B12	C18-C60-C61	-2.67	107.30	113.97
3	A	800	B12	O34-C32-C31	-2.65	113.29	121.07
4	C	801	DCA	C6P-C5P-N4P	2.65	120.88	116.42
3	C	800	B12	C2R-C3R-C4R	2.64	107.90	103.22
4	C	801	DCA	O5P-C5P-N4P	-2.63	118.05	123.01
3	C	800	B12	O8R-C5R-C4R	-2.63	102.27	111.29
3	A	800	B12	C10-C11-N23	-2.60	119.98	124.43
3	A	800	B12	O63-C61-N62	-2.57	115.49	122.50
3	C	800	B12	C25-C2-C1	2.51	117.57	113.78
4	C	801	DCA	C6A-C5A-C4A	2.51	120.55	117.18
4	A	801	DCA	O9A-P3B-O7A	2.50	120.45	110.68
3	A	800	B12	C7B-C6B-C5B	-2.47	116.13	119.67
4	C	801	DCA	C4A-N9A-C1B	2.46	132.46	126.59
3	C	800	B12	C8-C9-N22	2.44	115.64	110.77
3	A	800	B12	C48-C13-C12	-2.41	109.88	116.63
3	C	800	B12	C37-C7-C6	2.38	114.62	107.12
3	A	800	B12	C7-C6-N22	2.38	112.29	107.94
3	A	800	B12	C7B-C8B-C9B	2.37	125.33	122.52
4	A	801	DCA	CAP-C9P-N8P	2.37	121.29	116.58
4	C	801	DCA	O2B-C2B-C3B	2.36	117.88	111.17
4	A	801	DCA	CEP-CBP-CCP	2.33	112.04	108.23
4	C	801	DCA	CDP-CBP-CAP	-2.33	104.78	108.82
4	A	801	DCA	N9A-C8A-N7A	2.32	117.08	113.91
3	C	800	B12	C26-C2-C3	2.28	111.45	107.41
3	C	800	B12	C41-C8-C7	-2.28	107.86	114.14
3	C	800	B12	C17-C18-C19	2.26	105.82	102.36
3	C	800	B12	C10-C9-N22	2.25	128.31	125.73
4	A	801	DCA	CDP-CBP-CCP	2.24	111.89	108.23
3	C	800	B12	C1-C19-C18	-2.23	118.23	121.88
3	C	800	B12	C5R-C4R-C3R	-2.22	107.78	114.85
3	C	800	B12	C10-C11-N23	-2.21	120.64	124.43
4	C	801	DCA	C6A-C5A-N7A	-2.21	127.90	132.02
3	A	800	B12	C4B-C5B-C6B	2.21	122.83	119.67
3	A	800	B12	O5-P-O3	2.20	115.47	106.78
4	A	801	DCA	CEP-CBP-CDP	2.19	113.63	109.17
3	C	800	B12	C6M-C6B-C5B	-2.18	116.26	120.74
3	A	800	B12	C2R-C3R-C4R	2.18	107.08	103.22
3	A	800	B12	C20-C1-N21	2.17	113.83	110.27
3	A	800	B12	O6R-C1R-N1B	2.15	112.29	108.06
3	C	800	B12	C7-C6-C5	-2.13	124.72	128.07
3	A	800	B12	C15-C16-N24	2.13	125.49	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C56-C55-C17	-2.13	111.42	115.52
3	C	800	B12	C5M-C5B-C4B	2.12	123.40	119.49
3	C	800	B12	C36-C7-C37	2.12	114.29	110.80
3	A	800	B12	C9-C10-C11	-2.11	122.91	125.97
3	A	800	B12	C3-C4-N21	2.10	114.60	111.97
4	A	801	DCA	O9P-C9P-N8P	-2.09	118.51	122.99
4	A	801	DCA	C6P-C7P-N8P	2.07	116.08	111.90
3	C	800	B12	C1-C19-N24	-2.00	103.98	106.24

There are no chirality outliers.

All (28) torsion outliers are listed below:

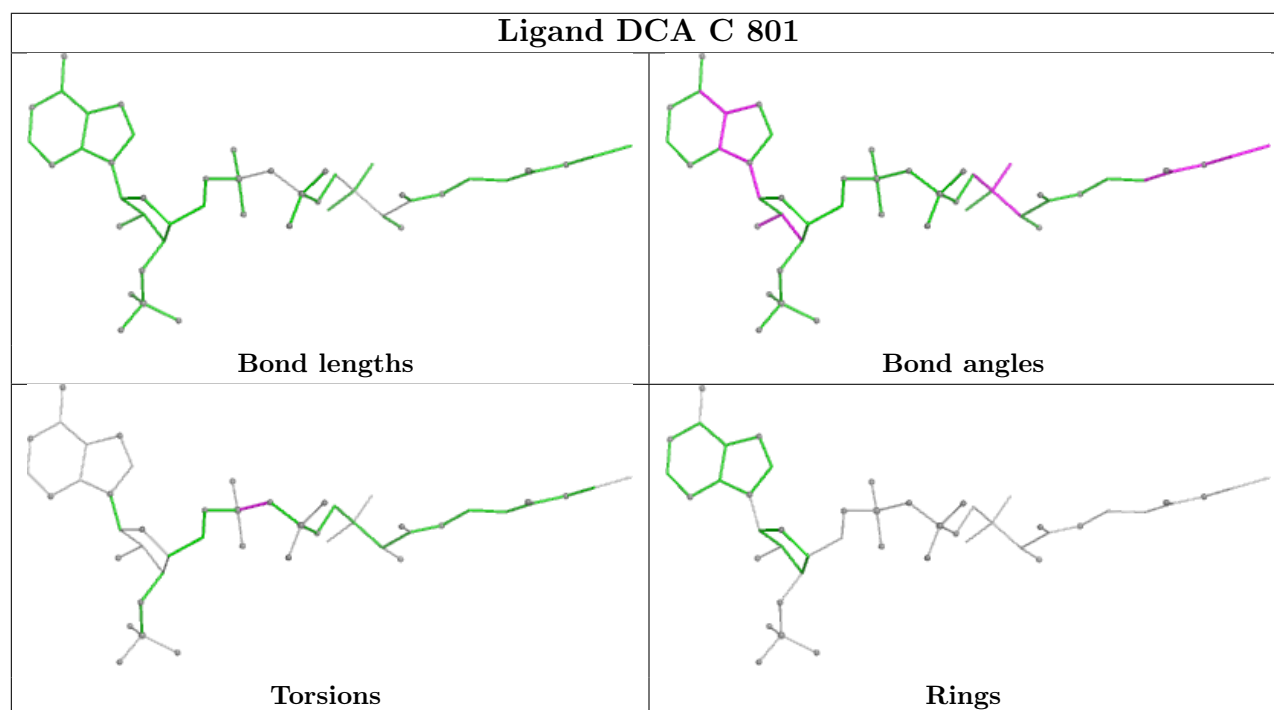
Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C16-C17-C55-C56
3	A	800	B12	C2R-C1R-N1B-C8B
3	C	800	B12	C2R-C1R-N1B-C8B
3	A	800	B12	C30-C31-C32-O34
3	A	800	B12	C30-C31-C32-N33
3	A	800	B12	C2P-O3-P-O2
3	A	800	B12	C42-C41-C8-C7
3	A	800	B12	C41-C42-C43-O44
3	A	800	B12	C41-C42-C43-N45
3	C	800	B12	C41-C42-C43-O44
3	C	800	B12	C41-C42-C43-N45
4	C	801	DCA	P2A-O3A-P1A-O1A
3	A	800	B12	C3-C30-C31-C32
4	A	801	DCA	P1A-O3A-P2A-O6A
3	A	800	B12	O6R-C1R-N1B-C8B
3	C	800	B12	O6R-C1R-N1B-C8B
4	A	801	DCA	P2A-O3A-P1A-O2A
3	C	800	B12	C2P-O3-P-O2
3	C	800	B12	C3-C30-C31-C32
3	C	800	B12	C42-C41-C8-C7
4	C	801	DCA	P2A-O3A-P1A-O2A
3	C	800	B12	C30-C31-C32-N33
4	A	801	DCA	P2A-O3A-P1A-O1A
3	A	800	B12	C55-C56-C57-O58
3	C	800	B12	C30-C31-C32-O34
3	A	800	B12	C55-C56-C57-N59

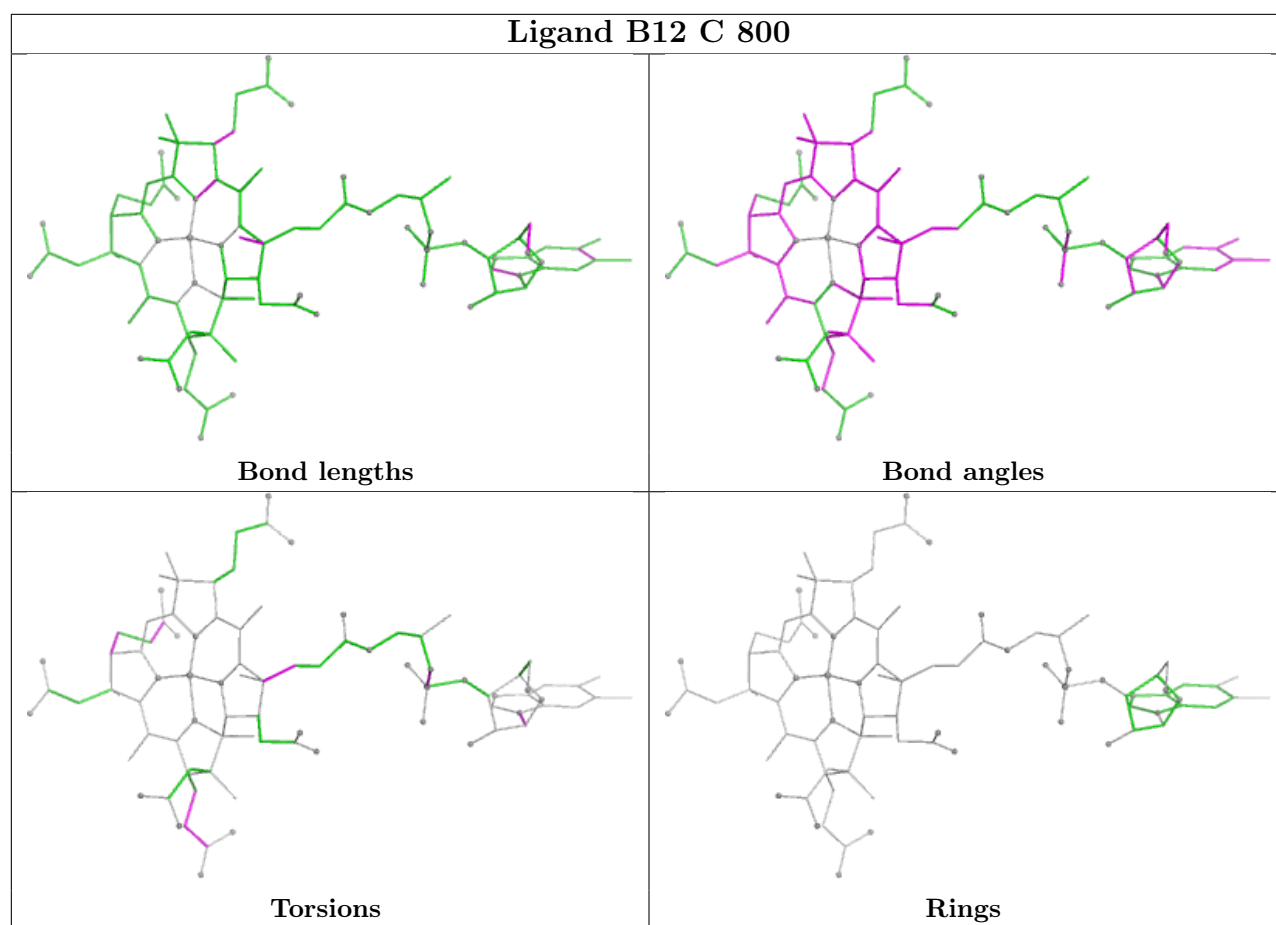
There are no ring outliers.

2 monomers are involved in 32 short contacts:

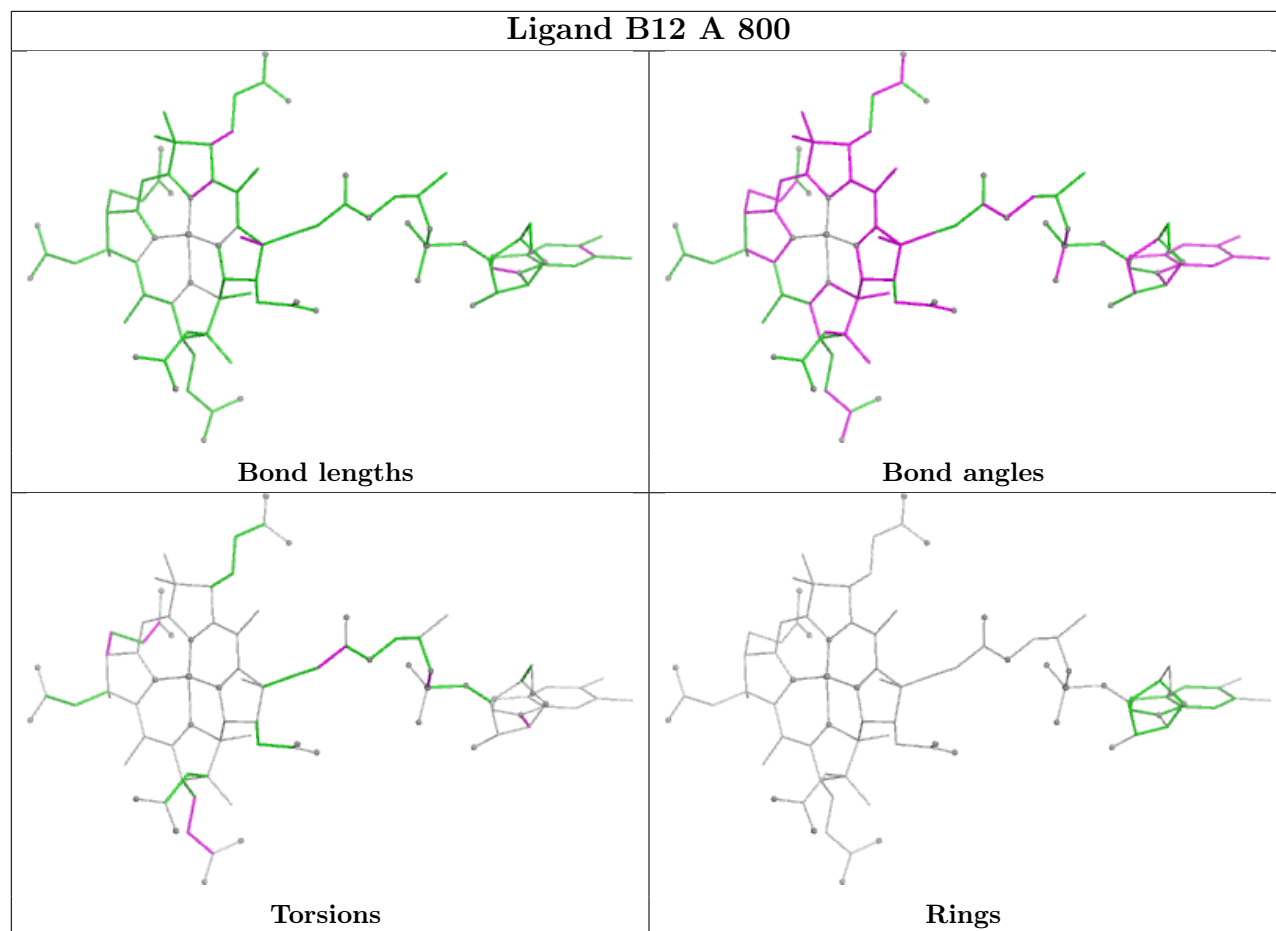
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	800	B12	16	0
3	A	800	B12	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

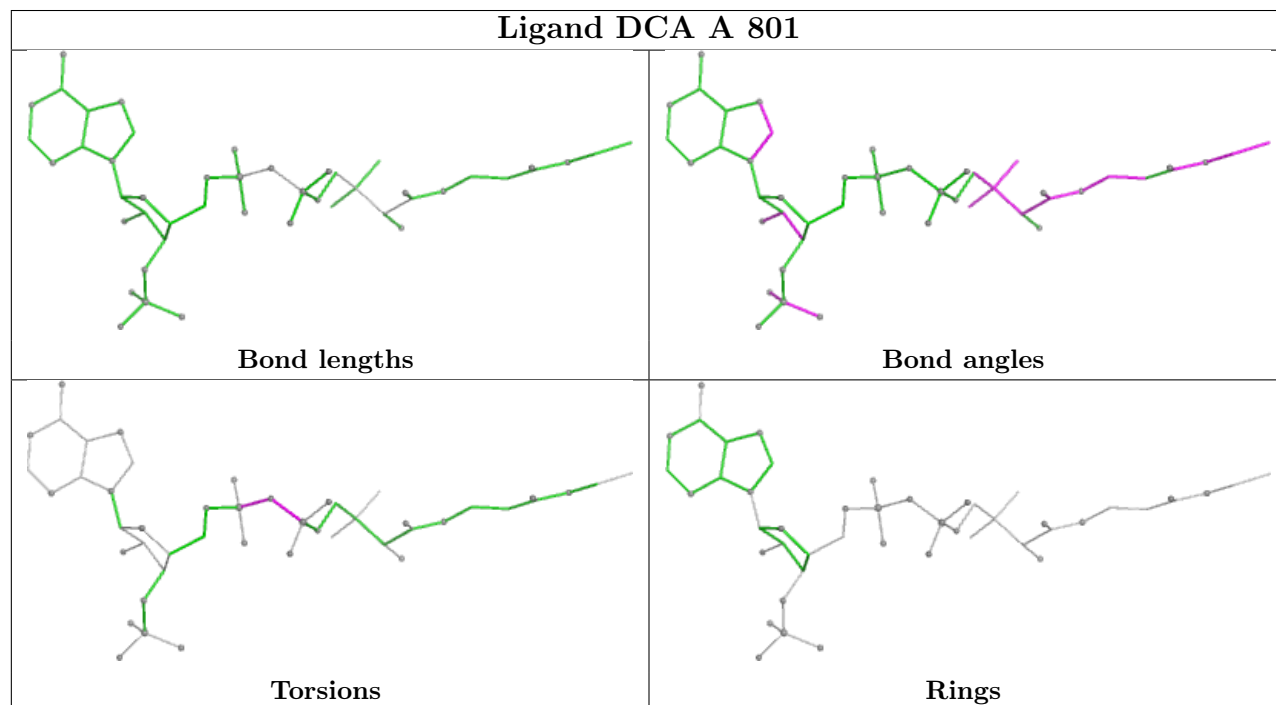




Ligand B12 A 800



Ligand DCA A 801



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/727 (100%)	-0.67	3 (0%) 88 86	17, 36, 64, 145	0
1	C	727/727 (100%)	-0.45	6 (0%) 82 80	20, 41, 74, 145	0
2	B	619/637 (97%)	-0.34	4 (0%) 85 83	21, 49, 74, 103	0
2	D	619/637 (97%)	0.18	21 (3%) 48 43	27, 58, 88, 112	0
All	All	2692/2728 (98%)	-0.34	34 (1%) 75 71	17, 45, 80, 145	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	107	TRP	3.8
2	D	107	TRP	3.8
2	D	20	THR	3.3
2	D	224	LEU	3.3
1	C	4	LEU	3.0
2	D	225	ALA	2.9
2	D	273	ALA	2.9
2	D	241	TYR	2.8
1	A	728	ALA	2.7
2	D	106	ALA	2.7
1	A	3	THR	2.6
2	D	230	ASP	2.6
2	D	146	ALA	2.5
2	D	217	LEU	2.4
2	B	106	ALA	2.4
2	D	93	PHE	2.4
2	D	277	PHE	2.4
2	D	234	VAL	2.4
2	D	176	ALA	2.4
2	D	305	ALA	2.3
1	A	2	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	105	ASP	2.3
2	D	216	VAL	2.2
1	C	5	PRO	2.2
1	C	576	ASN	2.2
2	D	281	ASN	2.2
1	C	23	ARG	2.1
2	D	262	TYR	2.1
1	C	2	SER	2.1
2	D	276	ALA	2.1
2	B	146	ALA	2.0
2	D	299	ALA	2.0
1	C	25	PHE	2.0
2	D	430	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

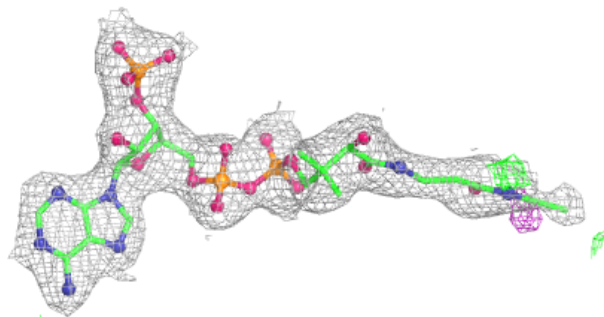
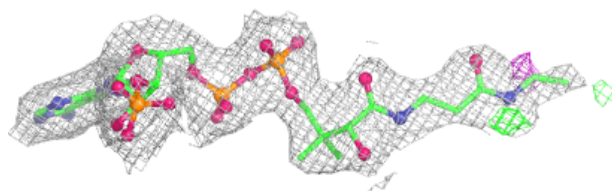
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DCA	C	801	47/47	0.97	0.06	21,28,32,35	0
3	B12	C	800	91/91	0.98	0.05	18,28,39,41	0
4	DCA	A	801	47/47	0.98	0.06	19,29,35,39	0
3	B12	A	800	91/91	0.98	0.05	13,27,35,38	0

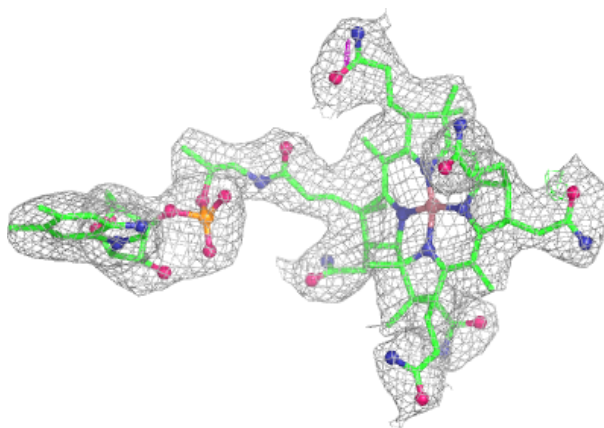
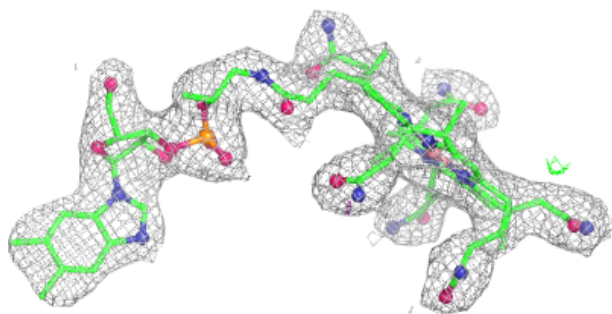
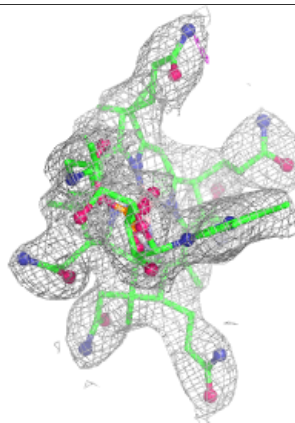
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DCA C 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

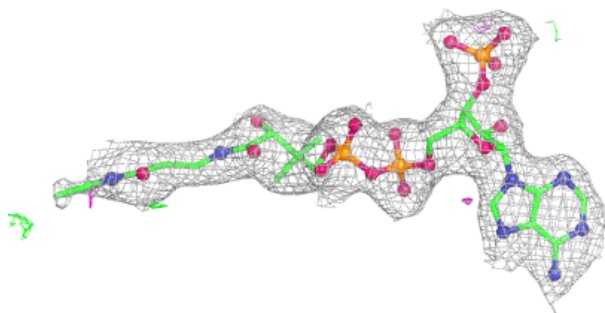
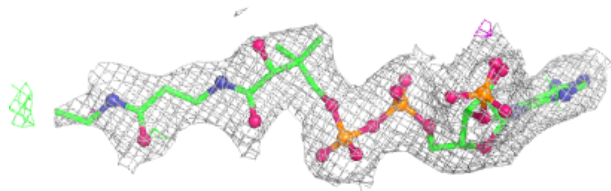
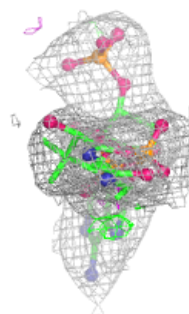
**Electron density around B12 C 800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

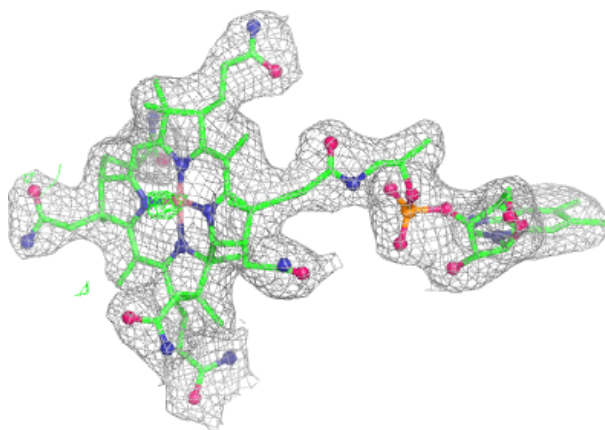
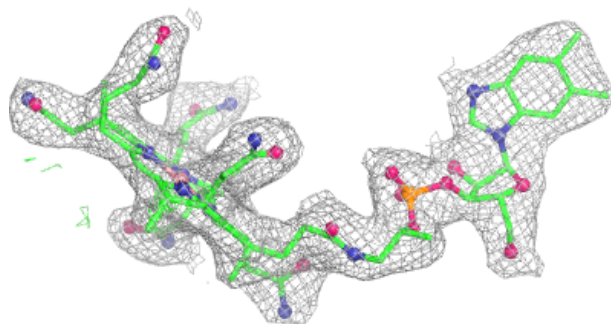
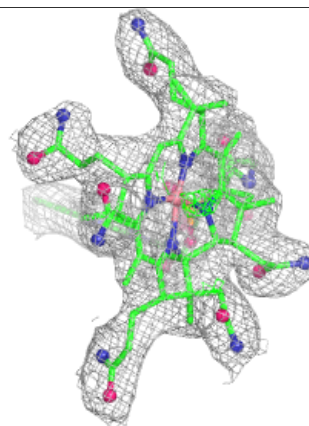


Electron density around DCA A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B12 A 800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.