



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:06 PM UTC

PDB ID : 6REQ / pdb\_00006req  
Title : METHYLMALONYL-COA MUTASE, 3-CARBOXYPROPYL-COA INHIBITOR COMPLEX  
Authors : Evans, P.R.; Mancina, F.  
Deposited on : 1998-09-03  
Resolution : 2.20 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

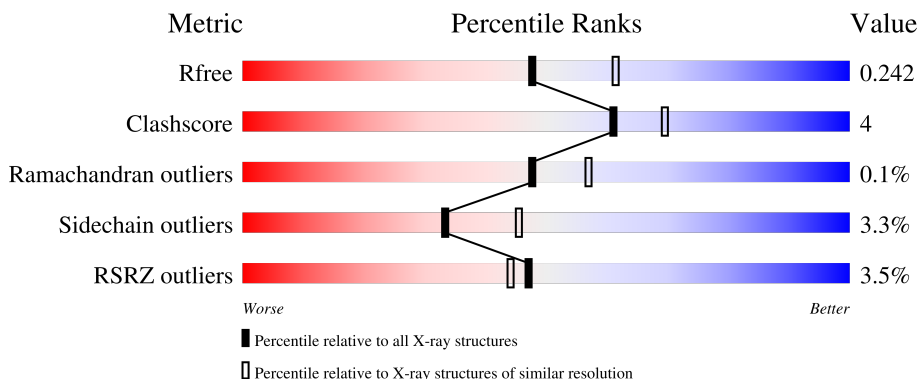
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	 45% 50% . .
1	C	727	 45% 48% 6%
2	B	637	 47% 45% 5% .
2	D	637	 46% 43% 7% . .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22116 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 PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	Total 5601	C 3538	N 971	O 1068	S 24	0	0	0
1	C	727	Total 5601	C 3538	N 971	O 1068	S 24	0	0	0

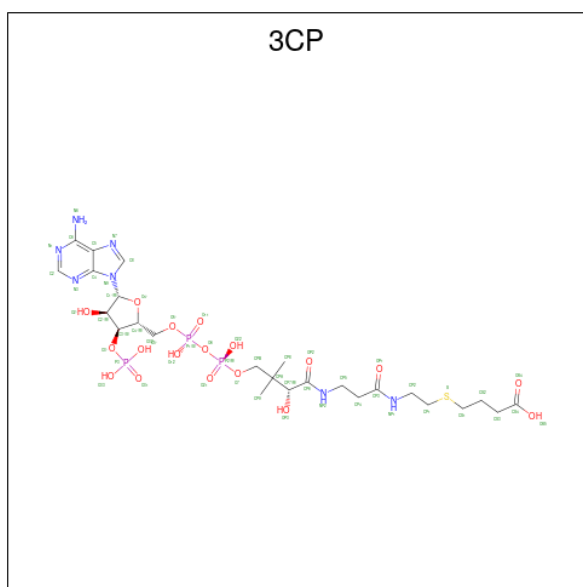
- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	Total 4731	C 2982	N 824	O 912	S 13	0	0	0
2	D	619	Total 4731	C 2982	N 824	O 912	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

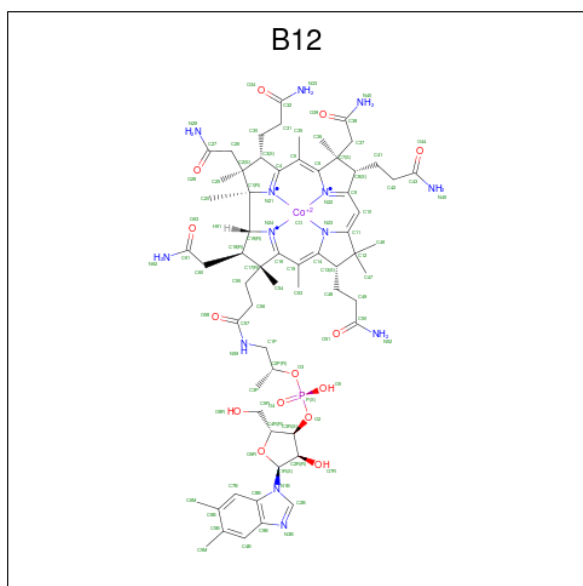
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is 3-CARBOXYPROPYL-COENZYME A (CCD ID: 3CP) (formula:  $C_{25}H_{42}N_7O_{18}P_3S$ ).



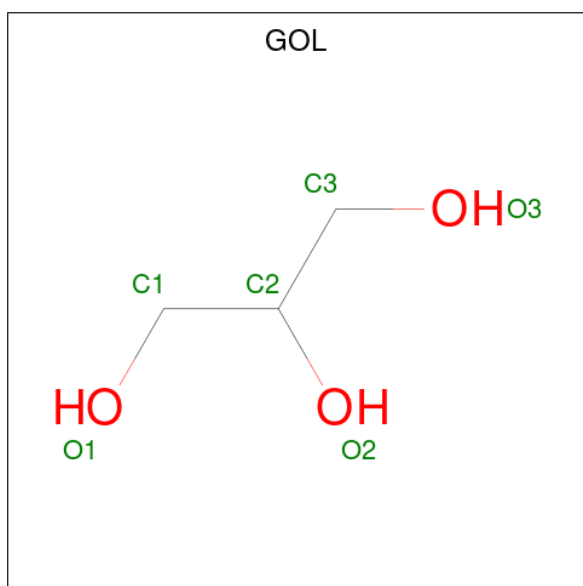
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	54	25	7	18	3	1	0	0
3	C	1	54	25	7	18	3	1	0	0

- Molecule 4 is COBALAMIN (CCD ID: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

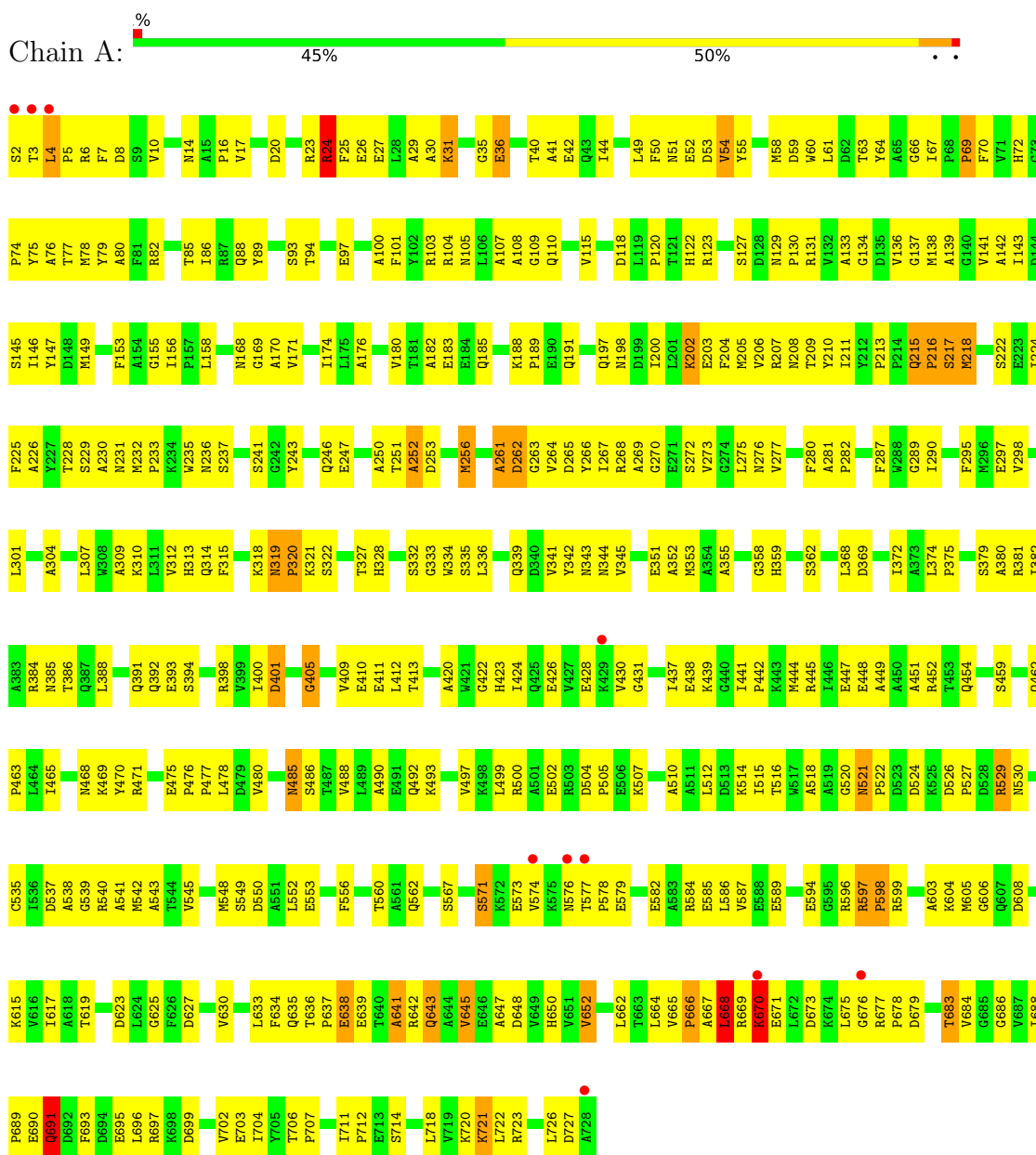
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	356	Total O 356 356	0	0
6	B	219	Total O 219 219	0	0
6	C	361	Total O 361 361	0	0
6	D	214	Total O 214 214	0	0

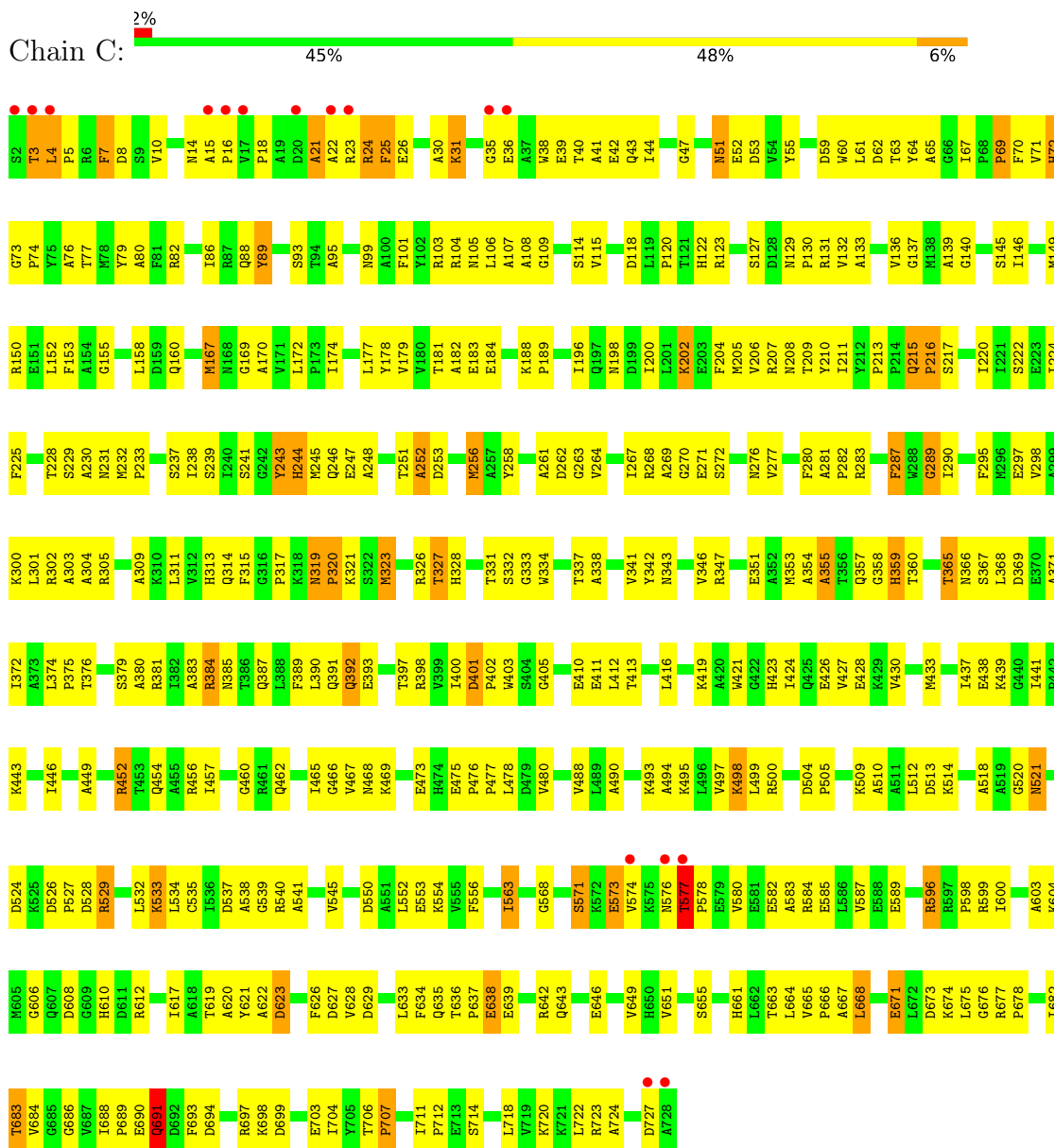
### 3 Residue-property plots [i](#)

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.

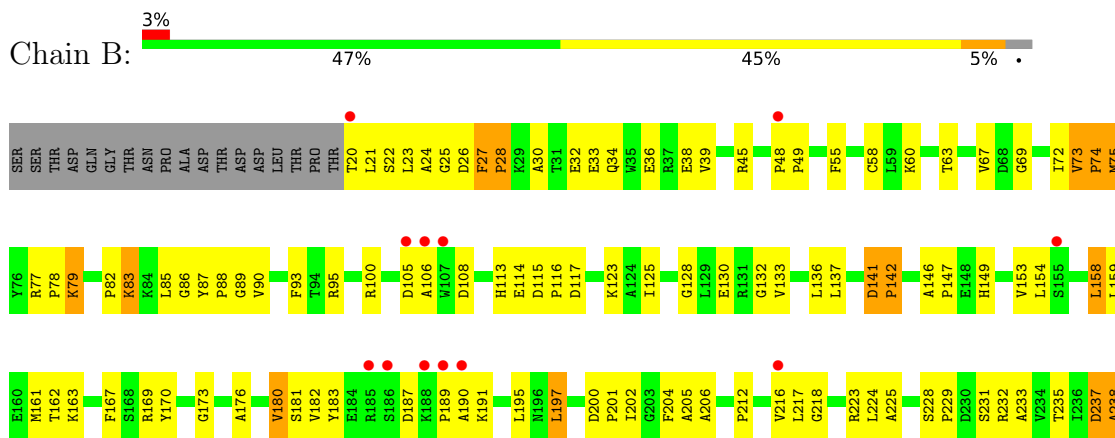
- Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE)

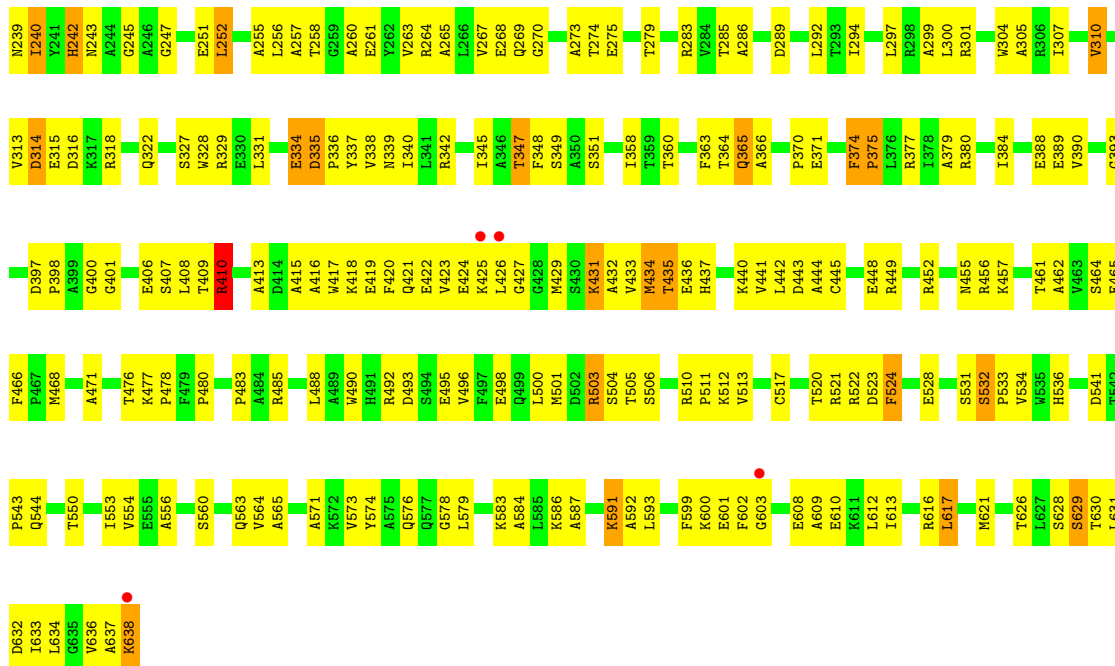


- Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE)

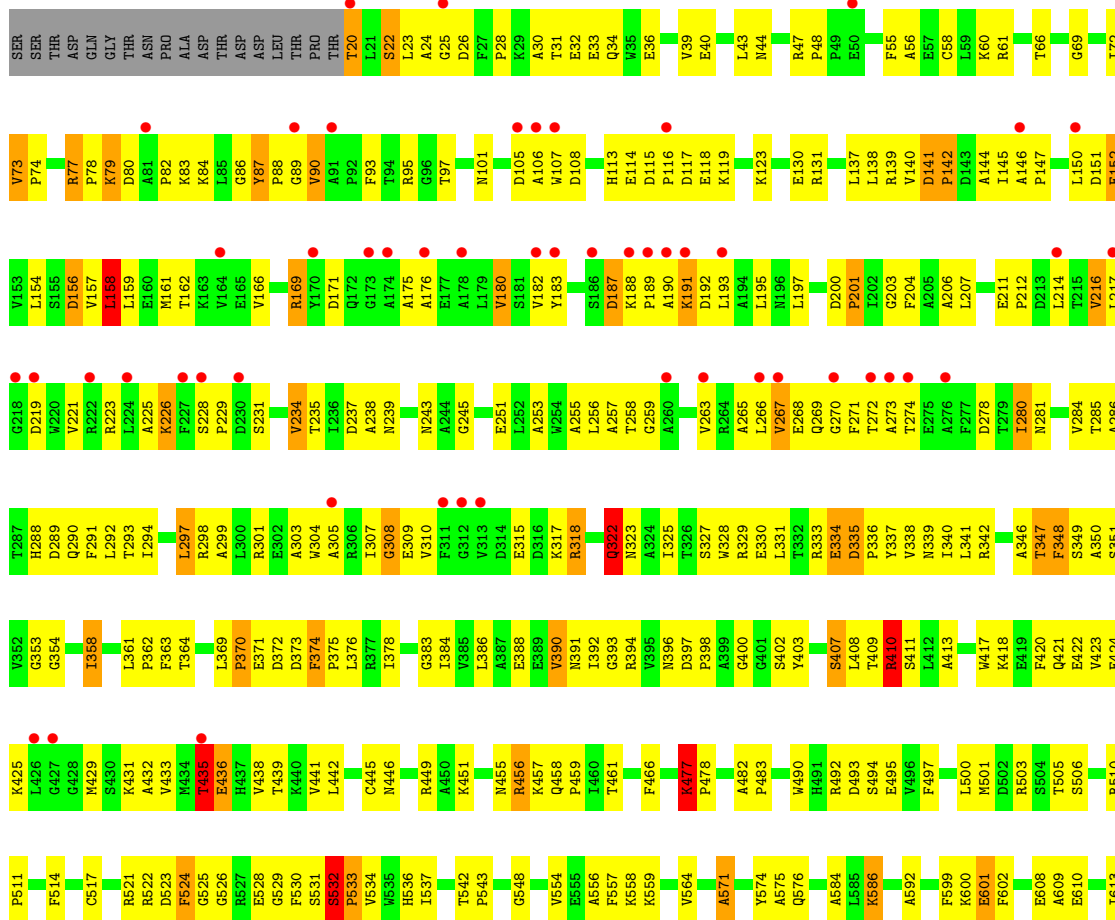


● Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)





● Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.95Å 160.46Å 88.48Å 90.00° 105.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.20) 98.7 (20.00-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.26 (at 2.19Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.206 , 0.263 0.195 , 0.242	Depositor DCC
$R_{free}$ test set	8160 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtrriage
Anisotropy	0.471	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 3CP, GOL, B12

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	1.11	3/5717 (0.1%)	2.83	628/7757 (8.1%)
1	C	1.15	4/5717 (0.1%)	2.85	661/7757 (8.5%)
2	B	1.00	5/4821 (0.1%)	2.75	530/6540 (8.1%)
2	D	1.03	7/4821 (0.1%)	2.81	504/6540 (7.7%)
All	All	1.08	19/21076 (0.1%)	2.81	2323/28594 (8.1%)

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	D	0	1
All	All	0	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	PHE	CA-CB	6.31	1.58	1.52
1	C	44	ILE	N-CA	-6.29	1.41	1.46
2	D	354	GLY	N-CA	-6.19	1.37	1.46
1	C	239	SER	N-CA	-5.87	1.38	1.47
2	B	289	ASP	N-CA	-5.86	1.39	1.46
1	A	171	VAL	N-CA	-5.70	1.40	1.46
2	D	87	TYR	CA-CB	5.68	1.64	1.54
2	B	410	ARG	NE-CZ	-5.42	1.27	1.33
2	D	90	VAL	N-CA	-5.38	1.39	1.46
2	D	270	GLY	N-CA	-5.33	1.38	1.45
2	B	410	ARG	CD-NE	-5.32	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	MET	N-CA	-5.29	1.39	1.46
2	D	86	GLY	N-CA	5.17	1.50	1.45
1	A	304	ALA	C-O	5.16	1.29	1.24
2	B	23	LEU	CA-C	-5.13	1.48	1.52
1	C	261	ALA	N-CA	5.07	1.52	1.46
2	B	87	TYR	CA-CB	5.06	1.63	1.54
1	C	42	GLU	N-CA	-5.04	1.39	1.46
2	D	530	PHE	N-CA	-5.03	1.40	1.46

All (2323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ARG	CD-NE-CZ	30.56	167.18	124.40
2	B	410	ARG	CD-NE-CZ	29.51	165.71	124.40
1	C	384	ARG	CD-NE-CZ	28.04	163.66	124.40
1	C	596	ARG	CD-NE-CZ	23.47	157.25	124.40
2	B	169	ARG	CD-NE-CZ	19.47	151.66	124.40
1	A	103	ARG	CD-NE-CZ	18.44	150.21	124.40
2	D	410	ARG	CD-NE-CZ	17.49	148.89	124.40
2	D	229	PRO	CA-C-N	16.63	143.90	120.29
2	D	229	PRO	C-N-CA	16.63	143.90	120.29
2	D	24	ALA	CA-C-N	16.56	140.99	120.13
2	D	24	ALA	C-N-CA	16.56	140.99	120.13
2	D	269	GLN	CA-C-N	16.53	147.69	120.91
2	D	269	GLN	C-N-CA	16.53	147.69	120.91
2	D	322	GLN	CB-CG-CD	15.07	138.23	112.60
2	D	89	GLY	CA-C-N	14.25	144.63	122.25
2	D	89	GLY	C-N-CA	14.25	144.63	122.25
2	B	86	GLY	CA-C-O	14.18	135.62	122.57
2	D	238	ALA	CA-C-N	13.89	141.43	120.31
2	D	238	ALA	C-N-CA	13.89	141.43	120.31
2	B	229	PRO	CA-C-N	13.75	139.82	120.29
2	B	229	PRO	C-N-CA	13.75	139.82	120.29
2	D	353	GLY	CA-C-N	13.54	140.56	120.11
2	D	353	GLY	C-N-CA	13.54	140.56	120.11
2	B	225	ALA	CA-C-N	13.49	138.75	120.54
2	B	225	ALA	C-N-CA	13.49	138.75	120.54
1	C	8	ASP	CA-C-N	13.36	142.41	121.98
1	C	8	ASP	C-N-CA	13.36	142.41	121.98
1	A	637	PRO	CA-C-N	13.14	138.31	120.44
1	A	637	PRO	C-N-CA	13.14	138.31	120.44
1	A	268	ARG	NE-CZ-NH2	-12.77	107.70	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	322	GLN	CA-C-O	12.38	134.07	120.70
1	A	553	GLU	CA-C-N	12.04	136.80	120.54
1	A	553	GLU	C-N-CA	12.04	136.80	120.54
1	C	314	GLN	O-C-N	-11.96	108.56	122.20
2	B	600	LYS	CA-C-N	11.72	137.16	120.28
2	B	600	LYS	C-N-CA	11.72	137.16	120.28
1	C	146	ILE	O-C-N	-11.71	110.42	121.89
1	A	333	GLY	CA-C-N	11.54	135.75	120.28
1	A	333	GLY	C-N-CA	11.54	135.75	120.28
1	C	146	ILE	CA-C-N	11.52	136.10	120.54
1	C	146	ILE	C-N-CA	11.52	136.10	120.54
1	A	313	HIS	CA-C-N	11.49	137.16	120.38
1	A	313	HIS	C-N-CA	11.49	137.16	120.38
1	A	520	GLY	O-C-N	-11.49	108.23	122.71
1	C	241	SER	N-CA-C	11.45	128.03	109.59
2	D	48	PRO	O-C-N	-11.34	116.09	121.31
2	D	255	ALA	N-CA-C	-11.17	99.07	111.14
1	C	633	LEU	CA-C-O	11.12	134.67	121.99
1	C	633	LEU	O-C-N	-11.04	109.18	122.65
2	B	93	PHE	CA-C-N	10.93	135.30	120.54
2	B	93	PHE	C-N-CA	10.93	135.30	120.54
1	A	170	ALA	CA-C-N	10.91	134.30	120.56
1	A	170	ALA	C-N-CA	10.91	134.30	120.56
2	B	86	GLY	O-C-N	-10.88	110.17	122.68
2	D	48	PRO	CA-C-O	10.82	128.69	120.90
1	C	62	ASP	CA-C-O	10.78	133.83	121.32
2	B	466	PHE	O-C-N	-10.78	116.57	121.53
1	C	276	ASN	CA-C-N	10.75	135.69	120.53
1	C	276	ASN	C-N-CA	10.75	135.69	120.53
1	A	673	ASP	CA-C-N	10.74	134.40	120.44
1	A	673	ASP	C-N-CA	10.74	134.40	120.44
1	A	343	ASN	O-C-N	-10.72	109.68	122.22
1	A	343	ASN	CA-C-N	10.55	135.47	120.28
1	A	343	ASN	C-N-CA	10.55	135.47	120.28
1	C	574	VAL	N-CA-CB	10.43	124.77	112.15
2	D	72	ILE	CB-CG1-CD1	10.39	135.63	113.80
1	C	476	PRO	N-CA-CB	10.38	109.00	103.19
1	C	319	ASN	CA-C-N	10.37	130.68	119.28
1	C	319	ASN	C-N-CA	10.37	130.68	119.28
2	B	89	GLY	CA-C-N	10.35	137.62	122.71
2	B	89	GLY	C-N-CA	10.35	137.62	122.71
1	C	52	GLU	CA-C-N	10.21	139.01	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	GLU	C-N-CA	10.21	139.01	121.14
1	C	55	TYR	N-CA-C	10.15	124.92	112.54
1	C	573	GLU	CA-C-O	-10.11	110.39	121.00
1	C	304	ALA	O-C-N	-10.10	111.42	122.12
1	C	16	PRO	CA-C-N	-10.09	112.52	123.02
1	C	16	PRO	C-N-CA	-10.09	112.52	123.02
2	D	26	ASP	CA-CB-CG	10.07	122.67	112.60
2	B	72	ILE	CB-CG1-CD1	10.07	134.95	113.80
1	C	676	GLY	CA-C-O	10.05	131.45	119.19
2	D	315	GLU	CA-C-N	10.04	140.73	122.06
2	D	315	GLU	C-N-CA	10.04	140.73	122.06
2	D	187	ASP	CA-C-N	10.03	144.63	122.67
2	D	187	ASP	C-N-CA	10.03	144.63	122.67
1	A	24	ARG	CG-CD-NE	10.01	134.03	112.00
2	B	601	GLU	O-C-N	-10.00	110.52	122.22
1	C	216	PRO	CA-C-N	10.00	133.44	120.44
1	C	216	PRO	C-N-CA	10.00	133.44	120.44
2	D	327	SER	N-CA-C	9.99	124.85	109.96
1	A	277	VAL	CA-C-N	9.98	136.57	120.60
1	A	277	VAL	C-N-CA	9.98	136.57	120.60
2	B	294	ILE	CA-C-N	9.98	133.65	120.28
2	B	294	ILE	C-N-CA	9.98	133.65	120.28
2	B	268	GLU	CA-C-N	9.97	139.21	122.65
2	B	268	GLU	C-N-CA	9.97	139.21	122.65
2	D	32	GLU	CA-C-N	9.96	133.63	120.28
2	D	32	GLU	C-N-CA	9.96	133.63	120.28
2	D	273	ALA	CA-C-N	9.95	133.62	120.28
2	D	273	ALA	C-N-CA	9.95	133.62	120.28
1	C	319	ASN	CA-C-O	9.95	130.46	119.32
2	B	32	GLU	CA-C-N	9.95	133.61	120.28
2	B	32	GLU	C-N-CA	9.95	133.61	120.28
1	C	664	LEU	CA-C-N	9.92	128.27	120.33
1	C	664	LEU	C-N-CA	9.92	128.27	120.33
1	A	8	ASP	CA-C-N	9.91	138.02	122.26
1	A	8	ASP	C-N-CA	9.91	138.02	122.26
1	C	320	PRO	CA-C-N	9.90	136.45	120.60
1	C	320	PRO	C-N-CA	9.90	136.45	120.60
1	A	232	MET	CA-C-N	9.90	129.66	119.56
1	A	232	MET	C-N-CA	9.90	129.66	119.56
1	A	676	GLY	CA-C-O	9.86	129.61	118.96
2	B	435	THR	CA-CB-CG2	9.85	127.25	110.50
1	C	410	GLU	CA-C-O	-9.83	110.00	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	HIS	CA-C-N	9.82	134.72	120.38
1	C	313	HIS	C-N-CA	9.82	134.72	120.38
1	A	82	ARG	CD-NE-CZ	9.82	138.15	124.40
1	C	727	ASP	CA-C-N	9.81	139.37	121.70
1	C	727	ASP	C-N-CA	9.81	139.37	121.70
1	A	241	SER	N-CA-C	9.80	125.83	109.76
1	A	51	ASN	CA-C-N	9.78	136.25	120.60
1	A	51	ASN	C-N-CA	9.78	136.25	120.60
2	D	398	PRO	O-C-N	-9.77	111.01	122.24
1	C	170	ALA	CA-C-N	9.76	132.86	120.56
1	C	170	ALA	C-N-CA	9.76	132.86	120.56
1	C	82	ARG	CD-NE-CZ	9.76	138.06	124.40
1	A	333	GLY	O-C-N	-9.74	112.84	122.19
2	B	100	ARG	CD-NE-CZ	9.73	138.03	124.40
1	A	183	GLU	O-C-N	-9.71	111.82	122.12
2	B	339	ASN	CA-C-N	9.71	132.80	120.56
2	B	339	ASN	C-N-CA	9.71	132.80	120.56
2	B	89	GLY	O-C-N	-9.69	110.08	122.39
2	D	78	PRO	O-C-N	-9.68	111.11	122.24
1	A	553	GLU	O-C-N	-9.62	110.96	122.22
1	C	41	ALA	CA-C-N	9.62	140.22	121.18
1	C	41	ALA	C-N-CA	9.62	140.22	121.18
2	B	337	TYR	O-C-N	-9.60	110.99	122.22
1	A	643	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	A	437	ILE	O-C-N	-9.58	112.20	121.87
1	A	675	LEU	CA-C-N	9.58	136.75	122.10
1	A	675	LEU	C-N-CA	9.58	136.75	122.10
1	A	699	ASP	CA-CB-CG	9.56	122.17	112.60
1	A	633	LEU	O-C-N	-9.54	111.00	122.65
1	C	676	GLY	O-C-N	-9.53	111.04	122.38
2	B	78	PRO	CA-C-N	9.51	135.82	120.60
2	B	78	PRO	C-N-CA	9.51	135.82	120.60
1	C	35	GLY	CA-C-O	9.51	131.53	121.64
1	C	251	THR	O-C-N	-9.49	111.97	122.79
2	D	477	LYS	N-CA-CB	9.43	124.27	110.32
2	D	410	ARG	NE-CZ-NH1	9.38	130.88	121.50
2	D	600	LYS	O-C-N	-9.37	111.25	122.22
1	A	146	ILE	O-C-N	-9.36	112.41	121.87
1	A	49	LEU	CA-C-O	9.36	133.89	120.51
2	D	24	ALA	O-C-N	-9.34	110.78	122.27
2	D	48	PRO	N-CA-CB	9.32	108.41	103.19
1	A	500	ARG	NE-CZ-NH2	-9.31	110.82	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	536	HIS	O-C-N	-9.27	111.38	122.22
2	D	86	GLY	CA-C-O	9.26	129.83	122.52
2	B	77	ARG	CD-NE-CZ	9.23	137.32	124.40
2	B	115	ASP	CA-C-O	9.22	126.56	119.46
2	D	301	ARG	CA-C-O	-9.22	110.93	121.07
1	A	535	CYS	O-C-N	-9.22	110.94	122.27
2	D	616	ARG	CD-NE-CZ	9.19	137.27	124.40
1	C	678	PRO	CA-C-N	9.17	134.25	120.31
1	C	678	PRO	C-N-CA	9.17	134.25	120.31
2	D	449	ARG	CA-C-N	9.14	132.88	120.54
2	D	449	ARG	C-N-CA	9.14	132.88	120.54
1	C	327	THR	N-CA-C	9.13	123.92	109.50
1	A	262	ASP	CA-C-N	9.12	130.30	119.99
1	A	262	ASP	C-N-CA	9.12	130.30	119.99
1	C	268	ARG	O-C-N	-9.12	112.67	122.07
1	A	224	ILE	N-CA-C	-9.07	101.56	110.72
2	D	364	THR	CA-C-N	9.05	135.09	120.60
2	D	364	THR	C-N-CA	9.05	135.09	120.60
1	C	723	ARG	O-C-N	-9.05	112.75	122.07
2	D	363	PHE	CA-C-N	9.03	140.01	121.94
2	D	363	PHE	C-N-CA	9.03	140.01	121.94
2	D	600	LYS	CA-C-N	9.03	135.05	120.60
2	D	600	LYS	C-N-CA	9.03	135.05	120.60
1	A	97	GLU	CA-C-N	9.03	132.72	120.44
1	A	97	GLU	C-N-CA	9.03	132.72	120.44
2	B	255	ALA	CA-C-N	9.01	132.16	120.44
2	B	255	ALA	C-N-CA	9.01	132.16	120.44
1	A	633	LEU	CA-C-O	9.00	132.25	121.99
1	C	723	ARG	CD-NE-CZ	8.99	136.99	124.40
2	B	25	GLY	O-C-N	-8.98	112.67	122.73
1	C	333	GLY	CA-C-N	8.95	132.27	120.28
1	C	333	GLY	C-N-CA	8.95	132.27	120.28
1	C	222	SER	O-C-N	-8.92	112.67	122.12
2	B	601	GLU	CA-C-N	8.90	140.62	122.55
2	B	601	GLU	C-N-CA	8.90	140.62	122.55
2	D	339	ASN	CA-C-N	8.90	131.77	120.56
2	D	339	ASN	C-N-CA	8.90	131.77	120.56
1	C	369	ASP	CA-C-N	8.88	132.53	120.54
1	C	369	ASP	C-N-CA	8.88	132.53	120.54
2	D	305	ALA	CA-C-N	8.87	132.89	120.29
2	D	305	ALA	C-N-CA	8.87	132.89	120.29
1	A	333	GLY	CA-C-O	8.87	129.88	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	ASP	CA-C-O	8.85	128.76	120.09
1	A	676	GLY	O-C-N	-8.85	112.68	122.50
1	A	493	LYS	O-C-N	-8.85	112.61	122.08
1	A	535	CYS	CA-C-N	8.81	131.66	120.56
1	A	535	CYS	C-N-CA	8.81	131.66	120.56
1	C	79	TYR	CA-C-N	8.77	132.40	120.38
1	C	79	TYR	C-N-CA	8.77	132.40	120.38
1	C	379	SER	CA-C-N	8.76	133.63	120.31
1	C	379	SER	C-N-CA	8.76	133.63	120.31
1	A	261	ALA	O-C-N	-8.75	112.17	122.15
1	A	645	VAL	O-C-N	-8.75	113.33	121.91
1	C	123	ARG	CD-NE-CZ	8.75	136.65	124.40
2	D	424	GLU	CA-C-N	8.75	132.88	120.28
2	D	424	GLU	C-N-CA	8.75	132.88	120.28
1	C	438	GLU	O-C-N	-8.75	111.99	122.22
2	B	536	HIS	O-C-N	-8.73	111.04	122.39
1	A	268	ARG	NH1-CZ-NH2	8.72	130.64	119.30
2	D	339	ASN	O-C-N	-8.71	111.07	122.39
1	C	261	ALA	O-C-N	-8.71	112.22	122.15
2	B	524	PHE	CA-CB-CG	8.70	122.50	113.80
2	D	307	ILE	N-CA-C	-8.68	101.88	110.30
2	B	187	ASP	CA-C-N	8.67	139.56	122.40
2	B	187	ASP	C-N-CA	8.67	139.56	122.40
2	D	610	GLU	O-C-N	-8.64	113.11	122.09
1	A	319	ASN	CA-C-O	8.62	128.97	119.32
1	C	74	PRO	CB-CA-C	-8.60	99.12	111.68
1	C	539	GLY	O-C-N	-8.59	113.94	122.19
2	D	183	TYR	CA-C-N	8.57	133.34	120.31
2	D	183	TYR	C-N-CA	8.57	133.34	120.31
1	C	41	ALA	O-C-N	-8.57	112.43	122.20
2	D	418	LYS	O-C-N	-8.57	113.04	122.12
1	C	63	THR	CA-C-N	8.56	135.78	122.94
1	C	63	THR	C-N-CA	8.56	135.78	122.94
2	D	410	ARG	NE-CZ-NH2	-8.56	111.50	119.20
2	B	485	ARG	CD-NE-CZ	8.54	136.36	124.40
2	D	528	GLU	CA-C-N	8.54	130.82	120.14
2	D	528	GLU	C-N-CA	8.54	130.82	120.14
1	C	333	GLY	O-C-N	-8.54	113.91	122.19
1	C	51	ASN	OD1-CG-ND2	8.53	131.13	122.60
2	B	338	VAL	CA-C-N	8.52	132.55	120.28
2	B	338	VAL	C-N-CA	8.52	132.55	120.28
1	A	262	ASP	O-C-N	-8.49	113.26	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	PHE	CA-CB-CG	-8.49	105.31	113.80
2	B	574	TYR	CA-C-N	8.48	131.47	120.44
2	B	574	TYR	C-N-CA	8.48	131.47	120.44
1	A	35	GLY	CA-C-N	8.48	134.25	120.94
1	A	35	GLY	C-N-CA	8.48	134.25	120.94
1	C	723	ARG	CA-C-N	8.47	131.99	120.38
1	C	723	ARG	C-N-CA	8.47	131.99	120.38
1	C	232	MET	CA-C-O	8.47	129.79	121.32
2	D	435	THR	CA-CB-CG2	8.46	124.88	110.50
2	D	146	ALA	CA-C-O	8.46	129.92	120.70
1	A	641	ALA	CA-C-N	8.46	131.43	120.44
1	A	641	ALA	C-N-CA	8.46	131.43	120.44
1	A	727	ASP	CA-C-N	8.45	136.91	121.70
1	A	727	ASP	C-N-CA	8.45	136.91	121.70
2	D	616	ARG	NE-CZ-NH1	-8.45	113.05	121.50
1	A	281	ALA	O-C-N	-8.43	112.54	120.55
1	A	334	TRP	O-C-N	-8.43	113.19	122.12
1	C	89	TYR	CA-CB-CG	8.41	129.05	113.90
1	C	79	TYR	CA-C-O	8.41	129.72	119.38
1	A	374	LEU	CA-C-O	8.39	129.85	120.70
1	A	488	VAL	CB-CA-C	-8.39	101.23	111.97
1	C	314	GLN	CA-C-O	8.37	129.58	120.20
2	D	69	GLY	N-CA-C	8.36	126.48	115.36
2	D	162	THR	N-CA-C	8.36	122.78	107.99
2	D	349	SER	CA-C-N	8.35	132.15	120.29
2	D	349	SER	C-N-CA	8.35	132.15	120.29
2	D	90	VAL	CA-C-O	8.35	129.83	120.90
1	A	691	GLN	OE1-CD-NE2	-8.35	114.25	122.60
1	C	541	ALA	CA-C-N	8.34	134.75	122.74
1	C	541	ALA	C-N-CA	8.34	134.75	122.74
1	A	475	GLU	CA-C-O	8.34	125.49	119.32
1	A	398	ARG	N-CA-C	8.33	122.55	112.38
1	C	252	ALA	CA-C-N	8.33	132.12	120.29
1	C	252	ALA	C-N-CA	8.33	132.12	120.29
1	C	202	LYS	CA-C-N	8.33	131.26	120.44
1	C	202	LYS	C-N-CA	8.33	131.26	120.44
2	D	532	SER	O-C-N	-8.32	111.75	121.32
1	C	449	ALA	CA-C-N	8.32	132.11	120.29
1	C	449	ALA	C-N-CA	8.32	132.11	120.29
1	A	599	ARG	CD-NE-CZ	8.32	136.05	124.40
1	C	282	PRO	N-CA-CB	8.32	111.42	103.52
1	C	24	ARG	CG-CD-NE	8.30	130.26	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	GLU	CA-C-N	8.28	134.44	122.35
1	A	42	GLU	C-N-CA	8.28	134.44	122.35
1	C	462	GLN	CA-C-O	8.27	127.19	119.59
1	C	313	HIS	O-C-N	-8.25	113.37	122.12
2	B	339	ASN	O-C-N	-8.25	112.57	122.22
1	C	439	LYS	CA-C-N	8.24	137.12	120.80
1	C	439	LYS	C-N-CA	8.24	137.12	120.80
1	A	691	GLN	CB-CG-CD	8.23	126.60	112.60
2	D	634	LEU	CA-C-N	8.23	137.85	121.06
2	D	634	LEU	C-N-CA	8.23	137.85	121.06
2	D	84	LYS	CA-C-O	-8.23	111.46	120.43
2	D	251	GLU	CA-C-N	8.21	131.49	120.65
2	D	251	GLU	C-N-CA	8.21	131.49	120.65
2	D	574	TYR	CA-C-N	8.21	131.12	120.44
2	D	574	TYR	C-N-CA	8.21	131.12	120.44
1	A	678	PRO	CA-C-N	8.21	134.63	120.68
1	A	678	PRO	C-N-CA	8.21	134.63	120.68
1	C	184	GLU	CA-C-N	8.20	137.32	122.06
1	C	184	GLU	C-N-CA	8.20	137.32	122.06
1	C	683	THR	N-CA-CB	8.20	123.97	110.85
1	A	677	ARG	CA-C-N	8.19	128.88	120.04
1	A	677	ARG	C-N-CA	8.19	128.88	120.04
1	A	539	GLY	CA-C-N	8.19	132.75	120.31
1	A	539	GLY	C-N-CA	8.19	132.75	120.31
1	A	526	ASP	CA-C-N	8.18	128.12	119.05
1	A	526	ASP	C-N-CA	8.18	128.12	119.05
1	C	521	ASN	O-C-N	-8.18	114.06	121.34
1	C	70	PHE	O-C-N	-8.16	111.71	122.40
1	C	430	VAL	O-C-N	-8.16	112.37	122.57
1	C	524	ASP	CA-CB-CG	8.15	120.75	112.60
1	C	697	ARG	O-C-N	-8.15	113.67	122.07
2	B	424	GLU	CA-C-N	8.15	131.20	120.28
2	B	424	GLU	C-N-CA	8.15	131.20	120.28
2	B	238	ALA	CA-C-N	8.13	131.98	120.28
2	B	238	ALA	C-N-CA	8.13	131.98	120.28
1	A	381	ARG	NE-CZ-NH2	8.12	126.51	119.20
2	B	183	TYR	CA-C-N	8.12	131.97	120.28
2	B	183	TYR	C-N-CA	8.12	131.97	120.28
1	C	497	VAL	CA-C-N	8.11	131.15	120.28
1	C	497	VAL	C-N-CA	8.11	131.15	120.28
2	D	493	ASP	O-C-N	-8.10	112.74	122.22
1	A	127	SER	N-CA-C	8.09	122.25	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	LYS	O-C-N	-8.06	113.70	122.09
1	A	516	THR	CA-C-N	8.06	131.42	120.54
1	A	516	THR	C-N-CA	8.06	131.42	120.54
1	C	711	ILE	O-C-N	-8.06	115.26	120.42
1	A	476	PRO	N-CA-CB	8.06	107.70	103.19
1	C	636	THR	N-CA-C	-8.05	98.31	110.07
2	D	24	ALA	CA-C-O	8.06	129.23	119.97
1	A	185	GLN	CA-C-N	8.05	133.95	120.91
1	A	185	GLN	C-N-CA	8.05	133.95	120.91
2	D	522	ARG	CB-CA-C	-8.05	97.43	110.79
1	C	206	VAL	CA-CB-CG1	8.04	124.08	110.40
1	C	47	GLY	O-C-N	-8.04	116.44	122.71
1	C	612	ARG	CA-C-N	8.03	128.69	119.94
1	C	612	ARG	C-N-CA	8.03	128.69	119.94
1	C	319	ASN	O-C-N	-8.02	112.45	121.36
2	D	229	PRO	O-C-N	-8.02	111.12	122.35
2	D	449	ARG	O-C-N	-8.02	113.81	122.07
1	C	248	ALA	CA-C-N	8.00	135.02	122.30
1	C	248	ALA	C-N-CA	8.00	135.02	122.30
2	D	601	GLU	O-C-N	-7.99	112.00	122.39
1	C	467	VAL	CA-C-O	-7.99	113.91	120.70
1	A	30	ALA	O-C-N	-7.98	113.79	122.09
1	A	704	ILE	O-C-N	-7.98	114.74	123.20
2	D	456	ARG	O-C-N	-7.98	109.18	122.03
2	B	610	GLU	CA-C-N	7.97	131.76	120.28
2	B	610	GLU	C-N-CA	7.97	131.76	120.28
1	A	136	VAL	CA-C-O	7.97	130.79	120.98
1	A	115	VAL	N-CA-C	7.96	120.04	108.58
1	A	169	GLY	O-C-N	-7.96	112.36	122.70
2	B	229	PRO	O-C-N	-7.95	111.49	122.30
1	A	228	THR	O-C-N	-7.94	113.10	122.15
1	A	327	THR	N-CA-C	7.94	121.82	109.52
2	D	47	ARG	CA-C-O	7.94	126.17	119.66
2	D	223	ARG	O-C-N	-7.92	112.96	122.22
1	C	333	GLY	CA-C-O	7.92	129.05	120.66
2	B	141	ASP	CA-C-N	7.91	127.83	119.05
2	B	141	ASP	C-N-CA	7.91	127.83	119.05
2	B	108	ASP	N-CA-CB	-7.91	97.11	110.16
2	D	510	ARG	CA-C-O	7.91	126.36	119.71
2	B	466	PHE	CA-C-O	7.91	126.58	120.26
1	C	553	GLU	CA-C-N	7.91	130.87	120.28
1	C	553	GLU	C-N-CA	7.91	130.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	147	PRO	CA-C-N	7.90	132.32	120.31
2	D	147	PRO	C-N-CA	7.90	132.32	120.31
1	C	633	LEU	CA-C-N	7.90	135.46	123.05
1	C	633	LEU	C-N-CA	7.90	135.46	123.05
2	D	93	PHE	CA-C-N	7.89	131.76	120.79
2	D	93	PHE	C-N-CA	7.89	131.76	120.79
2	B	239	ASN	O-C-N	-7.89	112.99	122.22
2	D	95	ARG	CG-CD-NE	7.89	129.35	112.00
1	C	691	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	C	208	ASN	OD1-CG-ND2	7.87	130.47	122.60
1	A	118	ASP	CA-CB-CG	7.86	120.46	112.60
1	C	678	PRO	N-CA-CB	7.86	110.77	103.46
2	D	61	ARG	CD-NE-CZ	7.86	135.41	124.40
1	A	41	ALA	CA-C-N	7.86	136.91	121.58
1	A	41	ALA	C-N-CA	7.86	136.91	121.58
1	C	526	ASP	CA-C-N	7.86	127.78	119.05
1	C	526	ASP	C-N-CA	7.86	127.78	119.05
2	B	363	PHE	CA-CB-CG	7.85	121.65	113.80
1	C	469	LYS	CA-C-O	7.85	129.56	119.98
2	D	289	ASP	CA-CB-CG	-7.85	104.75	112.60
1	A	215	GLN	CB-CG-CD	7.85	125.94	112.60
1	C	52	GLU	O-C-N	-7.84	112.16	122.59
1	A	449	ALA	O-C-N	-7.83	113.82	122.12
2	D	455	ASN	O-C-N	-7.83	112.55	122.34
2	B	202	ILE	CA-C-N	7.82	128.83	119.99
2	B	202	ILE	C-N-CA	7.82	128.83	119.99
2	D	391	ASN	OD1-CG-ND2	7.82	130.42	122.60
2	B	28	PRO	N-CA-CB	7.82	110.15	103.35
1	C	40	THR	O-C-N	-7.82	113.11	122.65
1	A	104	ARG	NE-CZ-NH2	7.81	126.23	119.20
1	C	603	ALA	N-CA-C	7.81	122.36	109.95
1	A	41	ALA	O-C-N	-7.80	111.97	122.43
1	C	690	GLU	O-C-N	-7.79	113.31	122.20
1	C	466	GLY	O-C-N	-7.79	113.34	122.60
1	C	535	CYS	O-C-N	-7.79	113.27	122.15
1	A	351	GLU	O-C-N	-7.78	113.87	122.12
1	A	441	ILE	CA-C-N	7.78	127.33	119.24
1	A	441	ILE	C-N-CA	7.78	127.33	119.24
1	A	101	PHE	O-C-N	-7.78	114.06	122.07
1	A	438	GLU	O-C-N	-7.77	113.13	122.22
1	C	232	MET	CA-C-N	7.76	127.48	119.56
1	C	232	MET	C-N-CA	7.76	127.48	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	SER	CA-C-O	7.74	129.56	120.58
1	C	189	PRO	CA-C-N	7.73	131.42	120.28
1	C	189	PRO	C-N-CA	7.73	131.42	120.28
1	A	369	ASP	CA-C-N	7.73	130.97	120.38
1	A	369	ASP	C-N-CA	7.73	130.97	120.38
2	D	409	THR	N-CA-C	-7.73	102.80	111.07
1	A	209	THR	N-CA-CB	7.73	122.74	111.54
2	B	397	ASP	CA-C-N	7.72	128.43	119.47
2	B	397	ASP	C-N-CA	7.72	128.43	119.47
2	B	560	SER	CA-C-N	7.71	134.86	121.07
2	B	560	SER	C-N-CA	7.71	134.86	121.07
1	A	225	PHE	CA-CB-CG	7.70	121.50	113.80
2	B	55	PHE	CA-C-N	7.70	132.37	120.82
2	B	55	PHE	C-N-CA	7.70	132.37	120.82
2	B	465	GLU	CA-C-O	7.70	128.87	120.32
2	D	327	SER	CA-C-O	7.70	129.55	120.70
2	D	304	TRP	CA-C-N	7.68	132.34	120.82
2	D	304	TRP	C-N-CA	7.68	132.34	120.82
1	C	253	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	430	VAL	O-C-N	-7.68	112.97	122.57
2	B	48	PRO	CA-C-N	7.68	128.38	119.47
2	B	48	PRO	C-N-CA	7.68	128.38	119.47
1	A	89	TYR	CA-CB-CG	7.67	127.70	113.90
1	A	637	PRO	O-C-N	-7.67	112.33	122.22
2	B	146	ALA	CA-C-N	7.67	128.06	119.32
2	B	146	ALA	C-N-CA	7.67	128.06	119.32
1	C	95	ALA	CA-C-N	7.67	130.41	120.44
1	C	95	ALA	C-N-CA	7.67	130.41	120.44
2	D	180	VAL	N-CA-CB	7.66	120.96	110.54
2	B	417	TRP	O-C-N	-7.66	114.18	122.07
2	D	228	SER	CA-C-N	7.66	127.83	119.87
2	D	228	SER	C-N-CA	7.66	127.83	119.87
1	C	684	VAL	CA-C-O	7.65	128.00	120.27
2	B	616	ARG	CD-NE-CZ	7.65	135.11	124.40
1	A	232	MET	O-C-N	-7.64	114.49	121.37
2	B	465	GLU	O-C-N	-7.63	114.38	123.31
2	D	107	TRP	CA-C-O	7.63	131.58	121.89
2	D	390	VAL	O-C-N	-7.63	113.18	122.18
1	A	388	LEU	CA-C-N	7.62	130.35	120.44
1	A	388	LEU	C-N-CA	7.62	130.35	120.44
1	A	518	ALA	O-C-N	-7.62	114.22	122.07
2	B	283	ARG	N-CA-CB	7.62	122.85	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	432	ALA	CA-C-N	7.62	131.23	120.42
2	B	432	ALA	C-N-CA	7.62	131.23	120.42
1	C	556	PHE	N-CA-C	7.62	122.88	112.90
2	B	235	THR	N-CA-CB	7.61	123.28	110.87
2	D	338	VAL	O-C-N	-7.61	114.18	121.87
1	C	439	LYS	O-C-N	-7.61	111.33	122.43
1	A	662	LEU	CA-C-O	-7.59	111.52	120.10
1	A	666	PRO	N-CA-CB	7.59	111.35	103.23
2	D	397	ASP	CA-C-N	7.59	127.97	119.32
2	D	397	ASP	C-N-CA	7.59	127.97	119.32
1	C	343	ASN	O-C-N	-7.59	113.34	122.22
2	D	342	ARG	CA-C-O	-7.59	112.78	120.90
1	A	313	HIS	O-C-N	-7.58	113.56	122.20
1	A	545	VAL	CA-C-N	7.58	128.36	119.94
1	A	545	VAL	C-N-CA	7.58	128.36	119.94
1	C	528	ASP	CA-C-N	7.58	135.05	122.54
1	C	528	ASP	C-N-CA	7.58	135.05	122.54
2	D	116	PRO	N-CA-CB	7.58	111.34	103.23
2	D	558	LYS	O-C-N	-7.57	114.09	122.12
2	D	456	ARG	CA-C-O	7.57	128.82	120.12
2	B	239	ASN	CA-C-N	7.57	130.36	120.60
2	B	239	ASN	C-N-CA	7.57	130.36	120.60
1	A	690	GLU	O-C-N	-7.57	113.37	122.22
1	C	416	LEU	CA-C-O	-7.57	112.91	120.70
2	B	304	TRP	CA-C-O	-7.56	112.53	120.55
2	D	422	GLU	CA-C-N	7.56	131.16	120.42
2	D	422	GLU	C-N-CA	7.56	131.16	120.42
2	D	490	TRP	CA-C-N	7.55	133.41	122.77
2	D	490	TRP	C-N-CA	7.55	133.41	122.77
2	B	348	PHE	CA-CB-CG	7.54	121.34	113.80
1	A	690	GLU	CA-C-N	7.54	132.66	120.60
1	A	690	GLU	C-N-CA	7.54	132.66	120.60
1	C	509	LYS	O-C-N	-7.54	114.25	122.09
1	C	541	ALA	O-C-N	-7.54	112.67	122.39
1	A	146	ILE	CA-C-N	7.53	130.71	120.54
1	A	146	ILE	C-N-CA	7.53	130.71	120.54
1	A	574	VAL	N-CA-CB	7.53	121.26	112.15
2	B	228	SER	CA-C-N	7.53	127.17	119.56
2	B	228	SER	C-N-CA	7.53	127.17	119.56
1	A	198	ASN	N-CA-CB	-7.53	100.62	111.84
1	C	30	ALA	O-C-N	-7.53	114.14	122.12
1	C	520	GLY	O-C-N	-7.53	112.07	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	25	GLY	CA-C-O	-7.53	112.77	120.45
1	A	358	GLY	O-C-N	-7.52	110.82	122.18
1	A	439	LYS	CA-C-N	7.52	134.34	120.87
1	A	439	LYS	C-N-CA	7.52	134.34	120.87
1	A	576	ASN	N-CA-C	7.52	121.87	112.24
1	A	136	VAL	O-C-N	-7.52	114.62	122.66
1	C	149	MET	CA-C-N	7.52	130.35	120.28
1	C	149	MET	C-N-CA	7.52	130.35	120.28
2	B	419	GLU	CA-C-N	7.51	130.20	120.44
2	B	419	GLU	C-N-CA	7.51	130.20	120.44
1	C	711	ILE	CA-C-N	7.51	127.38	119.05
1	C	711	ILE	C-N-CA	7.51	127.38	119.05
1	C	398	ARG	N-CA-C	7.50	120.33	111.71
1	C	720	LYS	O-C-N	-7.50	114.29	122.09
1	C	72	HIS	CA-CB-CG	-7.49	106.31	113.80
1	C	433	MET	N-CA-C	7.48	119.08	111.07
2	B	197	LEU	N-CA-C	7.47	120.49	111.82
1	A	454	GLN	OE1-CD-NE2	7.47	130.07	122.60
1	A	603	ALA	N-CA-C	7.46	121.61	109.59
2	D	115	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	217	SER	CA-C-N	7.46	130.27	120.28
1	A	217	SER	C-N-CA	7.46	130.27	120.28
2	D	20	THR	O-C-N	-7.46	111.07	123.00
2	B	613	ILE	CA-C-O	7.45	129.37	120.65
1	A	550	ASP	O-C-N	-7.45	114.22	122.12
2	B	457	LYS	O-C-N	-7.44	113.12	122.27
2	D	166	VAL	N-CA-CB	7.43	124.93	112.44
2	B	190	ALA	CA-C-N	7.43	132.49	120.60
2	B	190	ALA	C-N-CA	7.43	132.49	120.60
1	C	707	PRO	N-CA-CB	7.43	109.79	103.25
2	D	400	GLY	CA-C-O	7.43	133.50	120.57
1	C	513	ASP	O-C-N	-7.43	114.25	122.12
2	B	267	VAL	O-C-N	-7.42	114.64	121.91
2	B	363	PHE	CA-C-N	7.42	135.82	122.38
2	B	363	PHE	C-N-CA	7.42	135.82	122.38
1	A	282	PRO	CA-C-N	7.42	133.99	122.49
1	A	282	PRO	C-N-CA	7.42	133.99	122.49
1	A	666	PRO	N-CA-C	-7.42	102.86	113.47
1	C	552	LEU	CA-C-N	7.42	130.22	120.28
1	C	552	LEU	C-N-CA	7.42	130.22	120.28
1	A	50	PHE	O-C-N	-7.41	114.55	123.29
1	A	451	ALA	O-C-N	-7.41	113.71	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	PRO	N-CA-CB	7.40	109.90	103.31
2	D	150	LEU	CA-C-N	7.40	130.06	120.44
2	D	150	LEU	C-N-CA	7.40	130.06	120.44
2	B	457	LYS	CA-C-N	7.39	133.94	123.30
2	B	457	LYS	C-N-CA	7.39	133.94	123.30
2	D	294	ILE	CA-C-N	7.39	130.18	120.28
2	D	294	ILE	C-N-CA	7.39	130.18	120.28
2	D	351	SER	CA-C-N	7.39	132.14	120.47
2	D	351	SER	C-N-CA	7.39	132.14	120.47
1	C	341	VAL	N-CA-C	7.38	120.27	111.05
2	B	351	SER	O-C-N	-7.38	114.47	122.07
1	C	25	PHE	CA-C-O	-7.37	113.11	120.70
1	C	40	THR	CA-C-N	7.37	131.13	120.38
1	C	40	THR	C-N-CA	7.37	131.13	120.38
2	B	511	PRO	N-CA-CB	7.36	109.75	103.35
1	C	282	PRO	CA-C-N	7.36	134.07	122.60
1	C	282	PRO	C-N-CA	7.36	134.07	122.60
1	C	283	ARG	NE-CZ-NH2	-7.36	112.58	119.20
1	C	691	GLN	CB-CG-CD	7.36	125.11	112.60
1	A	217	SER	O-C-N	-7.35	114.33	122.12
2	B	522	ARG	CB-CA-C	-7.35	98.19	110.68
2	B	204	PHE	O-C-N	-7.34	114.51	122.07
2	B	521	ARG	O-C-N	-7.34	114.34	122.12
1	C	412	LEU	CA-C-N	7.33	130.10	120.28
1	C	412	LEU	C-N-CA	7.33	130.10	120.28
1	C	320	PRO	N-CA-CB	7.33	111.30	103.39
2	B	60	LYS	O-C-N	-7.32	114.36	122.12
2	B	422	GLU	CA-C-N	7.32	129.78	120.56
2	B	422	GLU	C-N-CA	7.32	129.78	120.56
1	A	599	ARG	CG-CD-NE	7.31	128.09	112.00
1	C	204	PHE	CA-CB-CG	-7.30	106.50	113.80
2	B	255	ALA	N-CA-C	-7.30	103.26	111.14
2	B	500	LEU	N-CA-C	-7.30	103.41	111.36
1	A	394	SER	N-CA-C	7.29	119.23	111.28
1	A	339	GLN	O-C-N	-7.29	114.66	123.19
1	C	437	ILE	CA-C-O	-7.29	113.36	120.95
2	B	528	GLU	CA-C-N	7.29	128.07	119.98
2	B	528	GLU	C-N-CA	7.29	128.07	119.98
2	B	610	GLU	O-C-N	-7.29	112.90	122.59
2	D	285	THR	N-CA-C	7.29	121.72	110.20
2	B	327	SER	N-CA-C	7.28	120.80	109.96
2	D	466	PHE	O-C-N	-7.28	118.18	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200	ASP	CA-C-O	7.26	130.11	120.16
1	C	419	LYS	O-C-N	-7.26	114.59	122.07
1	A	156	ILE	CA-C-O	7.26	129.68	119.95
1	C	5	PRO	N-CA-CB	7.25	109.66	103.35
2	B	337	TYR	CA-C-N	7.25	131.93	120.47
2	B	337	TYR	C-N-CA	7.25	131.93	120.47
2	D	408	LEU	CA-C-N	7.25	129.86	120.44
2	D	408	LEU	C-N-CA	7.25	129.86	120.44
1	A	541	ALA	O-C-N	-7.24	112.38	122.37
1	C	475	GLU	CA-C-O	7.24	124.68	119.32
1	C	196	ILE	N-CA-C	-7.24	98.06	108.48
1	A	6	ARG	CD-NE-CZ	7.24	134.53	124.40
1	C	359	HIS	ND1-CE1-NE2	7.24	115.64	108.40
2	B	379	ALA	CA-C-O	-7.23	113.22	120.82
1	C	621	TYR	CA-C-O	-7.23	112.89	120.55
2	B	69	GLY	N-CA-C	7.22	126.01	114.90
1	A	319	ASN	CA-C-N	7.21	127.22	119.28
1	A	319	ASN	C-N-CA	7.21	127.22	119.28
2	B	307	ILE	CA-C-N	7.21	127.95	119.94
2	B	307	ILE	C-N-CA	7.21	127.95	119.94
1	A	341	VAL	N-CA-C	7.21	121.12	111.17
2	B	616	ARG	NE-CZ-NH2	7.21	125.69	119.20
2	D	115	ASP	CA-C-N	7.21	126.47	118.97
2	D	115	ASP	C-N-CA	7.21	126.47	118.97
2	D	601	GLU	CA-C-N	7.21	135.63	121.58
2	D	601	GLU	C-N-CA	7.21	135.63	121.58
1	C	468	ASN	OD1-CG-ND2	-7.20	115.40	122.60
2	D	372	ASP	CA-C-O	-7.20	113.45	120.94
1	C	622	ALA	CA-C-N	7.20	129.93	120.28
1	C	622	ALA	C-N-CA	7.20	129.93	120.28
2	B	125	ILE	CA-C-O	-7.20	113.54	121.17
1	C	673	ASP	CA-C-N	7.19	130.63	120.28
1	C	673	ASP	C-N-CA	7.19	130.63	120.28
2	D	263	VAL	N-CA-C	-7.19	103.17	111.00
1	A	524	ASP	CA-C-N	7.18	135.41	122.06
1	A	524	ASP	C-N-CA	7.18	135.41	122.06
2	D	44	ASN	OD1-CG-ND2	7.18	129.78	122.60
1	C	276	ASN	O-C-N	-7.17	114.67	122.85
1	C	224	ILE	N-CA-C	-7.17	103.79	110.53
1	C	8	ASP	CA-CB-CG	7.16	119.76	112.60
2	D	530	PHE	CA-C-N	7.16	130.46	120.29
2	D	530	PHE	C-N-CA	7.16	130.46	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	396	ASN	N-CA-CB	7.15	121.96	110.16
1	C	252	ALA	N-CA-C	7.15	119.08	111.28
2	B	461	THR	CA-C-O	7.15	128.75	120.96
1	C	389	PHE	O-C-N	-7.15	114.66	122.09
1	C	571	SER	CA-C-N	7.15	129.86	120.28
1	C	571	SER	C-N-CA	7.15	129.86	120.28
1	A	287	PHE	CA-CB-CG	7.15	120.95	113.80
1	A	579	GLU	CA-C-N	7.14	129.70	120.56
1	A	579	GLU	C-N-CA	7.14	129.70	120.56
1	C	38	TRP	CA-C-O	-7.14	112.55	120.69
1	A	688	ILE	CA-CB-CG1	7.13	122.52	110.40
1	A	277	VAL	O-C-N	-7.13	114.90	121.89
1	A	438	GLU	CA-C-N	7.13	133.62	121.14
1	A	438	GLU	C-N-CA	7.13	133.62	121.14
1	A	207	ARG	CD-NE-CZ	7.12	134.38	124.40
2	D	531	SER	N-CA-C	7.12	119.13	111.36
2	B	78	PRO	O-C-N	-7.12	113.03	122.64
1	C	577	THR	CA-C-O	7.12	127.49	120.23
1	A	23	ARG	O-C-N	-7.11	113.52	122.27
1	C	375	PRO	N-CA-CB	7.11	109.54	103.35
2	D	571	ALA	CA-C-N	7.11	130.13	120.54
2	D	571	ALA	C-N-CA	7.11	130.13	120.54
1	A	723	ARG	CA-C-N	7.10	130.11	120.38
1	A	723	ARG	C-N-CA	7.10	130.11	120.38
1	C	209	THR	N-CA-CB	7.10	121.83	111.54
1	C	610	HIS	CA-C-O	-7.10	113.21	121.16
2	B	146	ALA	CA-C-O	7.09	127.95	120.64
2	D	466	PHE	CA-C-O	7.09	125.93	120.26
1	C	297	GLU	CA-C-O	7.09	128.06	120.55
2	B	602	PHE	CA-C-N	7.09	135.30	121.41
2	B	602	PHE	C-N-CA	7.09	135.30	121.41
1	A	636	THR	N-CA-C	-7.08	99.73	110.07
2	B	85	LEU	CA-C-N	-7.08	111.79	122.06
2	B	85	LEU	C-N-CA	-7.08	111.79	122.06
2	D	26	ASP	CB-CA-C	-7.08	96.12	109.72
2	B	532	SER	CA-C-N	7.08	127.39	119.32
2	B	532	SER	C-N-CA	7.08	127.39	119.32
1	C	589	GLU	O-C-N	-7.08	114.62	122.12
1	A	69	PRO	CA-C-N	7.08	132.19	122.07
1	A	69	PRO	C-N-CA	7.08	132.19	122.07
2	B	377	ARG	O-C-N	-7.07	114.62	122.12
2	B	79	LYS	CA-C-N	7.07	135.36	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	79	LYS	C-N-CA	7.07	135.36	121.58
2	D	191	LYS	CA-C-N	7.07	132.66	120.58
2	D	191	LYS	C-N-CA	7.07	132.66	120.58
1	C	238	ILE	CA-C-N	7.06	134.12	123.24
1	C	238	ILE	C-N-CA	7.06	134.12	123.24
2	B	187	ASP	CA-C-O	7.05	130.59	120.51
2	B	531	SER	N-CA-C	7.05	119.04	111.36
1	C	351	GLU	O-C-N	-7.05	114.65	122.12
1	C	177	LEU	O-C-N	-7.04	113.98	122.22
1	C	334	TRP	O-C-N	-7.04	114.65	122.12
1	A	72	HIS	CB-CG-ND1	7.04	133.26	122.70
2	B	297	LEU	CA-C-N	7.04	130.29	120.29
2	B	297	LEU	C-N-CA	7.04	130.29	120.29
1	C	727	ASP	N-CA-CB	7.04	118.44	110.35
2	B	305	ALA	CA-C-N	7.03	129.71	120.28
2	B	305	ALA	C-N-CA	7.03	129.71	120.28
1	A	526	ASP	CA-C-O	7.01	126.96	120.09
2	D	119	LYS	N-CA-C	-7.01	103.25	111.03
1	C	443	LYS	O-C-N	-7.01	114.69	122.12
1	A	691	GLN	CA-CB-CG	7.00	128.10	114.10
1	A	556	PHE	N-CA-C	6.98	121.03	112.23
2	D	525	GLY	CA-C-N	6.98	127.69	119.94
2	D	525	GLY	C-N-CA	6.98	127.69	119.94
1	C	577	THR	CA-C-N	6.98	126.23	118.97
1	C	577	THR	C-N-CA	6.98	126.23	118.97
2	B	600	LYS	O-C-N	-6.98	113.31	122.39
2	D	48	PRO	CA-C-N	6.98	128.57	119.84
2	D	48	PRO	C-N-CA	6.98	128.57	119.84
2	D	203	GLY	O-C-N	-6.98	115.22	122.13
1	A	412	LEU	CA-C-N	6.97	129.51	120.44
1	A	412	LEU	C-N-CA	6.97	129.51	120.44
2	D	411	SER	O-C-N	-6.97	114.73	122.12
1	A	218	MET	CA-C-O	6.97	127.94	120.55
1	C	229	SER	CA-C-O	-6.97	113.10	120.63
2	B	132	GLY	N-CA-C	6.97	124.62	115.36
2	D	44	ASN	CA-CB-CG	-6.96	105.64	112.60
1	C	642	ARG	O-C-N	-6.96	114.74	122.12
1	A	206	VAL	CB-CA-C	-6.96	99.88	111.29
1	C	43	GLN	CA-C-O	6.96	129.61	120.98
1	C	504	ASP	CA-C-N	6.95	126.92	119.28
1	C	504	ASP	C-N-CA	6.95	126.92	119.28
1	A	275	LEU	CA-C-O	6.94	128.97	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620	ALA	O-C-N	-6.94	114.24	122.15
1	C	30	ALA	CA-C-N	6.94	129.58	120.28
1	C	30	ALA	C-N-CA	6.94	129.58	120.28
2	B	573	VAL	O-C-N	-6.94	115.14	121.87
1	A	537	ASP	CA-C-O	-6.93	113.55	120.82
2	D	420	PHE	CA-CB-CG	6.93	120.73	113.80
1	A	153	PHE	CA-CB-CG	-6.92	106.88	113.80
2	B	375	PRO	N-CA-CB	6.92	110.86	103.39
2	B	269	GLN	CA-C-N	6.91	133.44	121.07
2	B	269	GLN	C-N-CA	6.91	133.44	121.07
2	B	275	GLU	CA-C-N	6.91	129.84	120.44
2	B	275	GLU	C-N-CA	6.91	129.84	120.44
2	B	455	ASN	O-C-N	-6.91	112.83	122.37
1	C	258	TYR	O-C-N	-6.91	114.95	122.07
1	A	619	THR	O-C-N	-6.91	114.28	122.15
2	B	217	LEU	CA-C-N	6.91	127.77	120.03
2	B	217	LEU	C-N-CA	6.91	127.77	120.03
1	A	261	ALA	N-CA-C	-6.91	103.83	111.36
2	D	88	PRO	N-CA-CB	6.90	109.85	103.15
2	D	524	PHE	CA-CB-CG	6.90	120.70	113.80
2	B	270	GLY	N-CA-C	6.90	125.71	115.08
1	C	61	LEU	N-CA-C	6.90	121.31	112.34
2	B	36	GLU	O-C-N	-6.90	114.91	122.09
1	A	183	GLU	CA-C-N	6.90	132.24	120.72
1	A	183	GLU	C-N-CA	6.90	132.24	120.72
1	C	665	VAL	CA-C-N	6.90	126.70	119.05
1	C	665	VAL	C-N-CA	6.90	126.70	119.05
2	B	256	LEU	CA-C-N	6.89	129.52	120.28
2	B	256	LEU	C-N-CA	6.89	129.52	120.28
2	B	560	SER	O-C-N	-6.89	113.19	122.43
1	C	215	GLN	O-C-N	-6.89	113.40	121.32
1	C	283	ARG	NE-CZ-NH1	6.89	128.39	121.50
1	C	553	GLU	O-C-N	-6.89	114.82	122.12
1	A	105	ASN	CA-C-N	6.88	129.51	120.28
1	A	105	ASN	C-N-CA	6.88	129.51	120.28
1	A	393	GLU	N-CA-CB	-6.88	100.42	110.47
2	B	232	ARG	CD-NE-CZ	6.88	134.04	124.40
2	B	586	LYS	O-C-N	-6.88	114.98	122.07
1	C	107	ALA	O-C-N	-6.88	113.81	122.27
2	D	190	ALA	O-C-N	-6.88	114.93	122.09
2	D	195	LEU	CA-C-O	6.88	128.46	120.89
1	A	310	LYS	CA-C-O	-6.88	113.60	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ALA	CA-C-N	6.88	129.82	120.54
1	A	29	ALA	C-N-CA	6.88	129.82	120.54
1	A	678	PRO	CA-C-O	6.87	127.56	118.90
1	C	281	ALA	N-CA-CB	6.87	123.07	110.08
2	D	28	PRO	N-CA-CB	6.87	109.38	103.19
1	A	358	GLY	CA-C-N	6.86	132.51	122.63
1	A	358	GLY	C-N-CA	6.86	132.51	122.63
1	A	524	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	652	VAL	N-CA-CB	6.86	119.24	111.21
1	C	550	ASP	O-C-N	-6.86	114.33	122.15
1	C	576	ASN	N-CA-C	6.86	121.60	113.23
1	A	683	THR	N-CA-CB	6.85	122.29	111.20
2	D	609	ALA	O-C-N	-6.85	114.97	122.09
1	C	24	ARG	CD-NE-CZ	6.84	133.98	124.40
1	C	413	THR	CA-C-N	6.84	129.75	120.44
1	C	413	THR	C-N-CA	6.84	129.75	120.44
1	A	711	ILE	CA-C-N	6.84	126.65	119.05
1	A	711	ILE	C-N-CA	6.84	126.65	119.05
2	D	182	VAL	O-C-N	-6.84	115.10	121.94
1	C	220	ILE	CA-C-N	6.83	129.17	120.56
1	C	220	ILE	C-N-CA	6.83	129.17	120.56
2	D	223	ARG	CA-C-N	6.83	134.76	122.06
2	D	223	ARG	C-N-CA	6.83	134.76	122.06
1	A	393	GLU	N-CA-C	6.83	121.74	113.41
2	B	423	VAL	CA-C-N	6.82	129.31	120.44
2	B	423	VAL	C-N-CA	6.82	129.31	120.44
2	D	278	ASP	O-C-N	-6.82	113.52	122.59
1	C	167	MET	O-C-N	-6.82	114.80	123.26
2	D	113	HIS	O-C-N	-6.82	115.18	123.30
1	A	205	MET	O-C-N	-6.82	114.38	122.15
2	B	78	PRO	N-CA-CB	6.82	110.41	103.25
1	C	7	PHE	N-CA-C	6.82	121.45	113.20
1	A	608	ASP	CA-CB-CG	6.81	119.41	112.60
1	C	365	THR	O-C-N	-6.81	115.19	123.30
2	B	335	ASP	CA-CB-CG	6.81	119.41	112.60
1	C	59	ASP	N-CA-CB	-6.80	100.34	110.61
1	A	322	SER	O-C-N	-6.80	114.27	122.22
2	B	409	THR	N-CA-C	-6.79	103.80	111.07
1	A	213	PRO	CA-C-O	6.79	130.41	120.56
2	B	190	ALA	O-C-N	-6.79	115.03	122.09
1	A	282	PRO	O-C-N	-6.78	113.15	122.24
2	D	141	ASP	CA-C-N	6.78	126.73	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	141	ASP	C-N-CA	6.78	126.73	119.28
1	A	447	GLU	O-C-N	-6.78	114.94	122.12
1	C	225	PHE	CA-CB-CG	6.77	120.57	113.80
2	D	156	ASP	CA-C-N	6.76	130.82	122.37
2	D	156	ASP	C-N-CA	6.76	130.82	122.37
2	D	456	ARG	CA-C-N	6.76	132.98	121.14
2	D	456	ARG	C-N-CA	6.76	132.98	121.14
2	D	526	GLY	O-C-N	-6.76	115.69	122.18
2	D	79	LYS	O-C-N	-6.76	113.60	122.39
2	D	417	TRP	N-CA-C	-6.75	103.61	110.97
2	B	301	ARG	CA-C-O	-6.75	113.39	120.55
1	C	527	PRO	CA-C-N	6.74	131.38	120.60
1	C	527	PRO	C-N-CA	6.74	131.38	120.60
2	D	146	ALA	CA-C-N	6.74	126.69	119.28
2	D	146	ALA	C-N-CA	6.74	126.69	119.28
2	B	73	VAL	CA-C-N	6.74	126.37	119.56
2	B	73	VAL	C-N-CA	6.74	126.37	119.56
1	C	183	GLU	O-C-N	-6.74	115.08	122.09
2	D	235	THR	N-CA-CB	6.73	121.08	110.84
2	D	25	GLY	CA-C-N	6.73	134.58	122.06
2	D	25	GLY	C-N-CA	6.73	134.58	122.06
2	B	364	THR	CA-C-N	6.73	131.36	120.60
2	B	364	THR	C-N-CA	6.73	131.36	120.60
2	D	373	ASP	CA-CB-CG	6.73	119.33	112.60
2	D	169	ARG	CD-NE-CZ	6.72	133.81	124.40
2	B	289	ASP	CA-CB-CG	-6.72	105.88	112.60
1	A	328	HIS	N-CA-C	-6.72	100.01	110.42
2	B	113	HIS	CA-CB-CG	-6.72	107.08	113.80
2	D	131	ARG	CD-NE-CZ	6.72	133.80	124.40
1	C	529	ARG	N-CA-CB	-6.71	100.55	110.49
2	B	180	VAL	N-CA-CB	6.71	119.66	110.54
2	B	462	ALA	CA-C-N	6.70	134.04	121.97
2	B	462	ALA	C-N-CA	6.70	134.04	121.97
1	A	539	GLY	O-C-N	-6.70	115.76	122.19
2	D	446	ASN	CA-C-O	-6.70	112.53	120.10
1	A	309	ALA	CA-C-O	-6.70	113.79	120.82
2	B	191	LYS	CA-C-N	6.70	132.06	120.68
2	B	191	LYS	C-N-CA	6.70	132.06	120.68
1	C	338	ALA	CA-C-N	6.69	132.64	122.93
1	C	338	ALA	C-N-CA	6.69	132.64	122.93
1	C	198	ASN	CA-CB-CG	6.69	119.29	112.60
1	C	150	ARG	CB-CA-C	-6.69	99.69	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	GLN	OE1-CD-NE2	-6.69	115.91	122.60
2	D	337	TYR	O-C-N	-6.69	113.69	122.39
2	D	521	ARG	CA-C-N	6.69	129.25	120.28
2	D	521	ARG	C-N-CA	6.69	129.25	120.28
1	C	358	GLY	N-CA-C	-6.69	105.22	115.66
1	A	82	ARG	NE-CZ-NH1	6.69	128.19	121.50
1	A	392	GLN	N-CA-C	6.69	121.74	112.45
2	B	493	ASP	N-CA-C	6.69	119.40	111.71
2	D	77	ARG	CA-C-N	6.68	126.94	119.32
2	D	77	ARG	C-N-CA	6.68	126.94	119.32
1	A	169	GLY	CA-C-O	6.68	132.19	120.57
1	A	188	LYS	CA-C-N	6.68	126.46	119.05
1	A	188	LYS	C-N-CA	6.68	126.46	119.05
2	D	86	GLY	O-C-N	-6.68	114.59	122.87
1	A	211	ILE	N-CA-CB	6.67	122.24	111.23
1	A	677	ARG	CA-C-O	6.67	128.62	120.54
1	A	180	VAL	O-C-N	-6.67	114.96	121.90
2	D	610	GLU	CA-C-N	6.67	131.27	120.60
2	D	610	GLU	C-N-CA	6.67	131.27	120.60
2	B	243	ASN	CA-C-N	6.67	134.46	122.06
2	B	243	ASN	C-N-CA	6.67	134.46	122.06
2	B	501	MET	O-C-N	-6.67	115.05	122.12
2	B	374	PHE	CA-C-N	6.67	126.61	119.28
2	B	374	PHE	C-N-CA	6.67	126.61	119.28
2	D	117	ASP	CA-CB-CG	6.67	119.27	112.60
1	C	473	GLU	N-CA-C	-6.66	103.95	111.14
1	A	423	HIS	CA-CB-CG	6.66	120.46	113.80
1	C	539	GLY	CA-C-N	6.66	129.87	120.28
1	C	539	GLY	C-N-CA	6.66	129.87	120.28
1	A	381	ARG	O-C-N	-6.65	114.57	122.15
1	C	38	TRP	N-CA-C	-6.65	99.19	109.76
1	C	105	ASN	CA-CB-CG	-6.65	105.95	112.60
2	B	268	GLU	O-C-N	-6.64	115.08	122.12
2	D	158	LEU	CA-C-N	6.64	129.85	120.28
2	D	158	LEU	C-N-CA	6.64	129.85	120.28
1	A	76	ALA	N-CA-C	6.64	118.52	111.28
2	D	423	VAL	CA-C-N	6.64	129.47	120.44
2	D	423	VAL	C-N-CA	6.64	129.47	120.44
1	A	712	PRO	CA-C-N	6.64	129.07	120.44
1	A	712	PRO	C-N-CA	6.64	129.07	120.44
1	C	636	THR	CA-C-N	6.64	126.58	119.28
1	C	636	THR	C-N-CA	6.64	126.58	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ALA	CA-C-N	6.63	129.17	120.28
1	A	30	ALA	C-N-CA	6.63	129.17	120.28
1	A	639	GLU	CA-C-N	6.63	129.06	120.44
1	A	639	GLU	C-N-CA	6.63	129.06	120.44
1	C	133	ALA	CA-C-N	6.63	132.60	120.79
1	C	133	ALA	C-N-CA	6.63	132.60	120.79
2	B	617	LEU	N-CA-C	-6.63	98.09	108.90
2	B	488	LEU	N-CA-C	6.63	119.98	110.24
1	A	55	TYR	N-CA-C	6.62	120.62	112.54
1	A	497	VAL	N-CA-C	-6.62	103.88	110.30
2	D	89	GLY	O-C-N	-6.62	113.98	122.39
1	A	270	GLY	O-C-N	-6.61	115.83	122.18
2	D	525	GLY	O-C-N	-6.61	115.58	122.13
1	C	231	ASN	O-C-N	-6.61	114.24	122.24
1	A	577	THR	CA-C-N	6.61	126.38	119.05
1	A	577	THR	C-N-CA	6.61	126.38	119.05
1	A	233	PRO	N-CA-CB	6.60	110.08	103.48
2	B	495	GLU	O-C-N	-6.60	115.12	122.12
2	D	238	ALA	O-C-N	-6.60	113.35	122.46
2	B	492	ARG	CD-NE-CZ	6.60	133.64	124.40
1	A	485	ASN	O-C-N	-6.60	115.13	122.12
1	A	410	GLU	CA-C-O	-6.59	113.56	120.55
1	C	424	ILE	O-C-N	-6.59	115.47	121.87
1	C	583	ALA	CA-C-N	6.59	129.01	120.44
1	C	583	ALA	C-N-CA	6.59	129.01	120.44
1	C	518	ALA	N-CA-CB	6.59	119.81	110.12
2	B	147	PRO	CA-C-N	6.59	131.72	120.72
2	B	147	PRO	C-N-CA	6.59	131.72	120.72
1	A	596	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	527	PRO	N-CA-CB	6.58	110.56	103.33
2	B	340	ILE	N-CA-CB	6.57	118.24	110.55
1	C	449	ALA	O-C-N	-6.57	115.15	122.12
1	C	145	SER	CA-C-N	6.57	129.80	120.53
1	C	145	SER	C-N-CA	6.57	129.80	120.53
1	C	385	ASN	CA-C-N	6.57	129.41	120.54
1	C	385	ASN	C-N-CA	6.57	129.41	120.54
1	A	40	THR	O-C-N	-6.57	114.64	122.65
1	C	400	ILE	CA-C-O	6.57	128.90	120.95
2	D	237	ASP	O-C-N	-6.56	113.35	122.41
2	B	483	PRO	N-CA-CB	6.56	109.02	103.25
1	C	268	ARG	NE-CZ-NH2	-6.56	113.30	119.20
2	B	449	ARG	O-C-N	-6.55	115.33	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	533	PRO	N-CA-CB	6.55	110.53	103.33
2	B	335	ASP	CA-C-N	6.54	126.17	119.56
2	B	335	ASP	C-N-CA	6.54	126.17	119.56
2	D	157	VAL	N-CA-C	6.53	118.22	108.23
1	A	726	LEU	N-CA-C	6.53	118.48	111.36
1	C	23	ARG	O-C-N	-6.53	114.24	122.27
2	D	558	LYS	CA-C-N	6.53	130.24	120.31
2	D	558	LYS	C-N-CA	6.53	130.24	120.31
1	C	79	TYR	O-C-N	-6.53	113.68	122.43
1	A	53	ASP	O-C-N	-6.52	114.59	122.22
1	C	469	LYS	O-C-N	-6.52	115.17	123.26
1	A	405	GLY	O-C-N	-6.52	114.23	122.70
2	B	218	GLY	O-C-N	-6.52	115.85	122.17
2	B	616	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	C	456	ARG	NE-CZ-NH2	6.52	125.06	119.20
2	D	315	GLU	N-CA-C	6.51	120.33	112.38
2	D	151	ASP	CA-C-O	-6.51	113.98	120.82
2	B	55	PHE	O-C-N	-6.51	115.11	122.08
1	C	337	THR	CA-C-O	6.51	129.44	121.56
1	C	699	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	368	LEU	CA-C-N	6.51	133.20	122.73
1	A	368	LEU	C-N-CA	6.51	133.20	122.73
2	B	283	ARG	CD-NE-CZ	6.51	133.51	124.40
1	A	318	LYS	CA-C-O	6.50	126.29	119.14
1	C	3	THR	N-CA-CB	6.50	121.48	110.49
1	C	167	MET	CA-C-O	6.50	127.91	119.98
1	C	638	GLU	CB-CG-CD	6.50	123.65	112.60
1	C	359	HIS	N-CA-C	6.50	120.05	111.28
1	C	277	VAL	O-C-N	-6.49	115.53	121.89
1	A	314	GLN	CA-C-N	6.49	134.24	121.58
1	A	314	GLN	C-N-CA	6.49	134.24	121.58
2	B	286	ALA	N-CA-C	-6.49	97.94	108.52
1	C	150	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	A	298	VAL	O-C-N	-6.49	115.58	121.87
1	A	269	ALA	O-C-N	-6.49	115.39	122.07
2	B	182	VAL	CA-C-N	6.49	128.97	120.28
2	B	182	VAL	C-N-CA	6.49	128.97	120.28
1	C	220	ILE	O-C-N	-6.49	115.45	121.94
1	C	412	LEU	O-C-N	-6.48	115.25	122.12
2	D	384	ILE	CA-C-O	6.48	127.72	120.85
1	C	287	PHE	CA-CB-CG	6.48	120.28	113.80
1	C	321	LYS	CA-C-N	6.48	129.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	LYS	C-N-CA	6.48	129.61	120.28
2	B	225	ALA	O-C-N	-6.48	114.64	122.22
2	D	506	SER	N-CA-C	6.48	119.16	111.71
1	C	35	GLY	O-C-N	-6.47	115.08	122.85
1	C	477	PRO	N-CA-CB	6.47	109.07	103.31
1	A	462	GLN	CA-C-O	6.47	125.54	119.59
2	B	476	THR	CA-CB-CG2	6.47	121.49	110.50
2	B	445	CYS	CA-C-N	6.46	128.94	120.28
2	B	445	CYS	C-N-CA	6.46	128.94	120.28
1	C	35	GLY	CA-C-N	6.46	132.73	120.97
1	C	35	GLY	C-N-CA	6.46	132.73	120.97
2	D	338	VAL	CA-C-N	6.46	130.94	120.60
2	D	338	VAL	C-N-CA	6.46	130.94	120.60
1	A	82	ARG	CA-C-O	6.46	125.81	119.22
1	C	723	ARG	CB-CG-CD	6.46	126.16	111.30
1	C	541	ALA	CA-C-O	6.46	127.24	119.43
2	D	243	ASN	O-C-N	-6.46	114.67	122.22
1	A	374	LEU	O-C-N	-6.45	114.43	121.53
2	B	21	LEU	CA-C-O	6.45	128.06	120.58
1	A	677	ARG	O-C-N	-6.45	114.72	121.04
1	C	381	ARG	O-C-N	-6.44	114.80	122.15
1	C	646	GLU	O-C-N	-6.44	115.29	122.12
1	C	237	SER	N-CA-C	6.44	120.97	113.18
2	B	418	LYS	O-C-N	-6.44	115.44	122.07
2	B	609	ALA	O-C-N	-6.44	115.39	122.09
2	D	633	ILE	O-C-N	-6.44	115.58	121.89
1	A	5	PRO	N-CA-CB	6.44	108.95	103.35
1	C	51	ASN	CA-CB-CG	-6.43	106.17	112.60
2	D	219	ASP	CA-CB-CG	-6.43	106.17	112.60
2	D	574	TYR	O-C-N	-6.43	115.30	122.12
2	B	421	GLN	CA-C-N	6.43	128.80	120.44
2	B	421	GLN	C-N-CA	6.43	128.80	120.44
1	C	71	VAL	O-C-N	-6.43	115.37	121.87
1	C	666	PRO	N-CA-CB	6.43	110.41	103.33
2	D	256	LEU	O-C-N	-6.43	115.45	122.07
1	A	539	GLY	CA-C-O	6.43	127.37	120.75
1	A	174	ILE	O-C-N	-6.42	115.61	121.91
1	C	629	ASP	N-CA-CB	6.42	120.63	110.55
2	B	123	LYS	O-C-N	-6.42	115.46	122.07
1	C	73	GLY	N-CA-C	-6.41	99.25	112.34
2	B	133	VAL	N-CA-C	-6.41	100.49	109.21
1	C	120	PRO	CA-C-N	6.41	128.77	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	PRO	C-N-CA	6.41	128.77	120.44
2	B	141	ASP	CA-CB-CG	6.41	119.01	112.60
2	B	181	SER	CA-C-O	-6.41	114.09	120.82
1	A	85	THR	CB-CA-C	-6.41	99.40	109.84
2	B	442	LEU	O-C-N	-6.40	115.33	122.12
1	C	514	LYS	O-C-N	-6.40	115.34	122.12
2	D	403	TYR	CA-C-O	6.39	127.53	120.82
2	B	478	PRO	N-CA-CB	6.39	108.87	103.25
1	C	608	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	444	MET	CA-C-O	6.38	127.19	120.42
2	B	191	LYS	O-C-N	-6.38	114.09	122.39
2	B	380	ARG	O-C-N	-6.38	114.87	122.15
2	B	204	PHE	CA-C-N	6.38	128.73	120.44
2	B	204	PHE	C-N-CA	6.38	128.73	120.44
2	B	524	PHE	CA-C-N	6.38	127.20	119.99
2	B	524	PHE	C-N-CA	6.38	127.20	119.99
2	B	531	SER	CA-C-O	6.38	127.18	120.42
1	C	535	CYS	CA-C-N	6.38	128.59	120.56
1	C	535	CYS	C-N-CA	6.38	128.59	120.56
2	B	269	GLN	O-C-N	-6.37	114.22	122.37
1	C	93	SER	N-CA-CB	-6.37	99.73	110.49
1	C	129	ASN	CA-C-N	6.37	126.58	119.32
1	C	129	ASN	C-N-CA	6.37	126.58	119.32
1	A	670	LYS	CG-CD-CE	6.37	125.94	111.30
1	A	633	LEU	CA-C-N	6.36	131.62	122.40
1	A	633	LEU	C-N-CA	6.36	131.62	122.40
1	A	101	PHE	CA-C-N	6.36	129.12	120.54
1	A	101	PHE	C-N-CA	6.36	129.12	120.54
1	A	231	ASN	CA-CB-CG	-6.36	106.24	112.60
2	B	229	PRO	N-CA-CB	6.36	109.61	103.51
1	C	88	GLN	OE1-CD-NE2	6.36	128.96	122.60
2	D	396	ASN	CA-C-O	6.36	127.72	120.54
2	D	191	LYS	O-C-N	-6.35	113.98	122.43
1	A	77	THR	CA-C-O	-6.35	112.06	119.05
1	C	571	SER	O-C-N	-6.35	115.39	122.12
2	D	182	VAL	CA-C-N	6.35	129.42	120.28
2	D	182	VAL	C-N-CA	6.35	129.42	120.28
2	D	511	PRO	N-CA-CB	6.35	108.87	103.35
1	C	371	ALA	CA-C-N	6.34	133.39	121.97
1	C	371	ALA	C-N-CA	6.34	133.39	121.97
1	A	344	ASN	CA-C-N	6.34	128.68	120.56
1	A	344	ASN	C-N-CA	6.34	128.68	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	ARG	CB-CA-C	-6.34	101.25	110.06
1	C	343	ASN	CA-C-N	6.34	129.41	120.28
1	C	343	ASN	C-N-CA	6.34	129.41	120.28
2	B	574	TYR	O-C-N	-6.34	115.40	122.12
1	C	82	ARG	CA-C-O	6.33	125.68	119.22
1	C	346	VAL	O-C-N	-6.33	115.31	121.90
2	D	144	ALA	CA-C-N	-6.33	112.37	122.50
2	D	144	ALA	C-N-CA	-6.33	112.37	122.50
2	B	267	VAL	CA-C-N	6.33	129.05	120.38
2	B	267	VAL	C-N-CA	6.33	129.05	120.38
2	D	626	THR	CA-C-O	-6.33	114.17	120.82
1	C	246	GLN	O-C-N	-6.33	115.55	122.07
1	A	410	GLU	CA-C-N	6.33	128.66	120.44
1	A	410	GLU	C-N-CA	6.33	128.66	120.44
1	C	177	LEU	CA-C-N	6.33	129.04	120.44
1	C	177	LEU	C-N-CA	6.33	129.04	120.44
1	A	272	SER	CA-C-N	6.32	132.69	122.76
1	A	272	SER	C-N-CA	6.32	132.69	122.76
2	D	337	TYR	CA-C-N	6.32	130.46	120.47
2	D	337	TYR	C-N-CA	6.32	130.46	120.47
1	A	63	THR	O-C-N	-6.32	113.66	122.76
1	C	341	VAL	O-C-N	-6.32	115.49	121.87
2	B	498	GLU	CA-C-N	6.31	129.90	120.31
2	B	498	GLU	C-N-CA	6.31	129.90	120.31
1	C	150	ARG	NH1-CZ-NH2	6.31	127.50	119.30
1	C	498	LYS	CA-CB-CG	6.30	126.71	114.10
1	C	184	GLU	O-C-N	-6.30	114.20	122.39
2	D	231	SER	CA-C-O	6.30	128.08	121.15
1	A	203	GLU	CA-C-O	-6.30	114.21	120.70
2	D	362	PRO	N-CA-CB	6.30	109.19	103.33
1	A	693	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	281	ALA	CA-C-N	6.29	125.98	119.56
1	A	281	ALA	C-N-CA	6.29	125.98	119.56
2	B	30	ALA	CA-C-O	6.29	128.21	121.16
1	A	49	LEU	O-C-N	-6.29	114.23	122.59
1	C	174	ILE	O-C-N	-6.29	115.36	121.90
2	D	417	TRP	O-C-N	-6.29	115.49	122.03
1	A	504	ASP	CA-C-O	6.29	123.38	119.29
1	A	721	LYS	CA-C-N	6.28	128.69	120.28
1	A	721	LYS	C-N-CA	6.28	128.69	120.28
1	C	108	ALA	O-C-N	-6.28	114.29	122.39
1	A	108	ALA	CA-C-N	6.28	131.71	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ALA	C-N-CA	6.28	131.71	122.10
1	C	314	GLN	CA-C-N	6.28	133.82	121.58
1	C	314	GLN	C-N-CA	6.28	133.82	121.58
1	A	424	ILE	CA-C-N	6.27	128.59	120.44
1	A	424	ILE	C-N-CA	6.27	128.59	120.44
1	C	359	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
1	A	627	ASP	N-CA-C	-6.27	98.52	108.73
2	B	200	ASP	CA-C-N	6.27	126.01	119.05
2	B	200	ASP	C-N-CA	6.27	126.01	119.05
2	D	557	PHE	CA-C-N	6.27	128.68	120.28
2	D	557	PHE	C-N-CA	6.27	128.68	120.28
1	C	627	ASP	N-CA-C	-6.27	99.00	108.96
1	A	189	PRO	CA-C-N	6.26	130.62	120.60
1	A	189	PRO	C-N-CA	6.26	130.62	120.60
1	C	488	VAL	N-CA-CB	6.26	118.59	110.57
2	B	338	VAL	O-C-N	-6.26	115.55	121.87
1	C	272	SER	CA-C-N	6.26	130.02	122.26
1	C	272	SER	C-N-CA	6.26	130.02	122.26
2	D	532	SER	CA-C-N	6.26	126.00	119.05
2	D	532	SER	C-N-CA	6.26	126.00	119.05
2	D	418	LYS	CA-C-O	-6.26	113.87	120.63
1	A	206	VAL	CA-CB-CG1	6.25	121.03	110.40
1	A	584	ARG	O-C-N	-6.25	115.63	122.07
1	A	702	VAL	CA-C-O	6.25	126.42	119.42
2	D	239	ASN	OD1-CG-ND2	6.25	128.85	122.60
2	B	406	GLU	CB-CG-CD	6.25	123.22	112.60
1	C	628	VAL	N-CA-C	6.25	116.92	108.17
2	B	384	ILE	O-C-N	-6.25	115.81	121.87
2	D	609	ALA	CA-C-N	6.25	128.97	120.54
2	D	609	ALA	C-N-CA	6.25	128.97	120.54
1	C	405	GLY	O-C-N	-6.24	116.16	122.65
1	A	594	GLU	N-CA-C	6.24	121.05	113.38
1	A	670	LYS	CA-CB-CG	-6.23	101.63	114.10
1	C	158	LEU	CA-C-N	6.23	132.05	121.14
1	C	158	LEU	C-N-CA	6.23	132.05	121.14
1	C	703	GLU	O-C-N	-6.23	116.29	123.33
1	C	466	GLY	CA-C-N	6.23	129.07	122.97
1	C	466	GLY	C-N-CA	6.23	129.07	122.97
2	B	159	LEU	N-CA-C	6.23	119.72	111.75
2	D	627	LEU	O-C-N	-6.23	115.66	122.07
1	C	198	ASN	N-CA-CB	-6.23	99.97	110.49
1	C	578	PRO	N-CA-CB	6.22	109.89	103.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	528	ASP	O-C-N	-6.22	114.30	122.39
2	D	204	PHE	CA-C-N	6.22	128.53	120.44
2	D	204	PHE	C-N-CA	6.22	128.53	120.44
2	B	631	LEU	CA-C-N	6.22	128.53	120.44
2	B	631	LEU	C-N-CA	6.22	128.53	120.44
1	C	79	TYR	N-CA-C	6.22	120.13	112.54
1	C	380	ALA	CA-C-N	6.22	129.12	120.29
1	C	380	ALA	C-N-CA	6.22	129.12	120.29
1	C	376	THR	N-CA-C	-6.22	100.78	110.17
2	B	455	ASN	CA-C-N	6.22	132.98	123.47
2	B	455	ASN	C-N-CA	6.22	132.98	123.47
1	C	244	HIS	CA-CB-CG	-6.21	107.58	113.80
1	C	270	GLY	CA-C-N	6.21	128.61	120.28
1	C	270	GLY	C-N-CA	6.21	128.61	120.28
1	C	232	MET	O-C-N	-6.21	116.28	121.12
2	D	159	LEU	N-CA-C	6.21	118.85	111.71
1	C	510	ALA	O-C-N	-6.21	115.68	122.07
2	B	170	TYR	N-CA-C	6.20	121.91	113.97
2	D	303	ALA	CA-C-O	-6.20	114.31	120.82
1	A	89	TYR	O-C-N	6.20	130.55	122.93
2	D	97	THR	N-CA-C	-6.20	103.22	111.96
1	C	172	LEU	O-C-N	-6.19	115.49	120.38
1	A	541	ALA	CA-C-N	6.19	133.36	121.54
1	A	541	ALA	C-N-CA	6.19	133.36	121.54
1	C	103	ARG	CD-NE-CZ	6.19	133.06	124.40
1	A	94	THR	CA-C-O	6.18	129.12	121.89
2	D	105	ASP	CA-CB-CG	-6.18	106.42	112.60
1	C	698	LYS	O-C-N	-6.18	114.99	122.22
1	A	295	PHE	CA-CB-CG	-6.17	107.62	113.80
2	D	394	ARG	NE-CZ-NH2	-6.17	113.64	119.20
1	A	61	LEU	N-CA-C	6.17	119.65	111.75
1	A	320	PRO	CA-C-N	6.17	129.16	120.28
1	A	320	PRO	C-N-CA	6.17	129.16	120.28
2	B	591	LYS	CA-CB-CG	6.17	126.44	114.10
2	B	360	THR	CA-C-N	-6.17	111.31	120.68
2	B	360	THR	C-N-CA	-6.17	111.31	120.68
1	C	118	ASP	CA-CB-CG	6.17	118.77	112.60
2	B	77	ARG	CA-C-N	6.17	127.55	119.84
2	B	77	ARG	C-N-CA	6.17	127.55	119.84
1	C	309	ALA	N-CA-C	-6.17	104.47	111.07
2	B	100	ARG	CA-C-O	-6.16	113.84	120.92
1	A	334	TRP	CA-C-N	6.16	131.00	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	TRP	C-N-CA	6.16	131.00	120.72
1	A	79	TYR	O-C-N	-6.15	114.18	122.43
1	A	720	LYS	CA-C-N	6.15	128.85	120.54
1	A	720	LYS	C-N-CA	6.15	128.85	120.54
1	A	488	VAL	N-CA-CB	6.15	117.75	110.55
1	C	416	LEU	N-CA-CB	6.15	118.99	110.07
2	D	225	ALA	CA-C-N	6.15	129.34	120.79
2	D	225	ALA	C-N-CA	6.15	129.34	120.79
2	B	410	ARG	NE-CZ-NH1	6.15	127.65	121.50
2	D	123	LYS	O-C-N	-6.15	115.50	122.08
1	A	375	PRO	N-CA-CB	6.15	108.78	103.31
1	A	447	GLU	CA-C-N	6.15	128.43	120.44
1	A	447	GLU	C-N-CA	6.15	128.43	120.44
2	D	371	GLU	CA-CB-CG	6.15	126.39	114.10
2	D	333	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	401	ASP	CA-C-N	6.14	125.86	119.05
1	A	401	ASP	C-N-CA	6.14	125.86	119.05
2	B	492	ARG	O-C-N	-6.14	115.61	122.86
1	A	120	PRO	CA-C-N	6.13	128.50	120.28
1	A	120	PRO	C-N-CA	6.13	128.50	120.28
1	A	133	ALA	O-C-N	-6.13	115.52	122.08
2	D	318	ARG	N-CA-C	6.13	120.62	113.20
1	C	31	LYS	CA-C-N	6.13	128.50	120.28
1	C	31	LYS	C-N-CA	6.13	128.50	120.28
2	D	425	LYS	CA-C-N	6.13	133.10	122.56
2	D	425	LYS	C-N-CA	6.13	133.10	122.56
1	A	683	THR	N-CA-C	-6.13	100.17	109.85
2	B	218	GLY	CA-C-N	6.13	128.41	120.44
2	B	218	GLY	C-N-CA	6.13	128.41	120.44
2	D	169	ARG	NE-CZ-NH2	-6.13	113.69	119.20
1	C	694	ASP	CA-C-N	6.12	128.49	120.28
1	C	694	ASP	C-N-CA	6.12	128.49	120.28
1	C	178	TYR	O-C-N	-6.12	115.48	122.09
1	A	448	GLU	O-C-N	-6.12	115.77	122.07
1	A	246	GLN	O-C-N	-6.12	115.77	122.07
1	A	213	PRO	O-C-N	-6.12	114.24	121.46
1	A	109	GLY	N-CA-C	6.12	124.57	115.64
1	C	723	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	C	131	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	A	332	SER	N-CA-C	6.11	118.57	109.59
2	D	407	SER	O-C-N	-6.11	115.78	122.07
1	A	210	TYR	N-CA-C	-6.10	102.90	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	GLU	O-C-N	-6.10	115.78	122.07
2	D	351	SER	O-C-N	-6.10	115.19	122.15
2	D	384	ILE	O-C-N	-6.10	115.54	121.83
1	C	44	ILE	N-CA-C	-6.10	101.07	107.60
1	C	300	LYS	CA-C-N	6.10	128.45	120.28
1	C	300	LYS	C-N-CA	6.10	128.45	120.28
1	C	704	ILE	CA-C-O	6.10	126.29	120.31
1	A	679	ASP	CA-C-O	-6.10	112.59	119.79
1	C	684	VAL	N-CA-CB	6.10	120.11	111.82
1	A	251	THR	N-CA-C	-6.09	102.32	110.55
1	A	647	ALA	N-CA-C	-6.09	104.47	113.61
1	A	60	TRP	CA-C-N	6.09	129.27	120.38
1	A	60	TRP	C-N-CA	6.09	129.27	120.38
2	B	147	PRO	O-C-N	-6.09	115.24	122.24
2	B	617	LEU	N-CA-CB	6.09	120.91	110.68
2	B	240	ILE	CA-C-N	6.09	128.94	120.29
2	B	240	ILE	C-N-CA	6.09	128.94	120.29
2	B	504	SER	CA-C-N	6.09	131.03	120.68
2	B	504	SER	C-N-CA	6.09	131.03	120.68
2	D	152	GLU	O-C-N	-6.09	115.67	122.12
1	C	22	ALA	CB-CA-C	6.08	120.94	110.84
2	D	123	LYS	CA-C-N	6.08	128.75	120.54
2	D	123	LYS	C-N-CA	6.08	128.75	120.54
1	A	409	VAL	N-CA-CB	6.08	117.66	110.55
2	B	158	LEU	CA-C-N	6.08	129.25	120.38
2	B	158	LEU	C-N-CA	6.08	129.25	120.38
1	C	222	SER	CA-C-N	6.08	129.54	120.31
1	C	222	SER	C-N-CA	6.08	129.54	120.31
1	C	724	ALA	O-C-N	-6.08	115.68	122.12
2	D	528	GLU	O-C-N	-6.08	115.22	122.15
2	B	398	PRO	N-CA-CB	6.07	110.10	103.30
2	D	304	TRP	O-C-N	-6.07	115.81	122.07
1	C	357	GLN	O-C-N	-6.07	113.57	122.43
1	A	226	ALA	O-C-N	-6.07	115.82	122.07
2	B	273	ALA	CA-C-N	6.06	128.40	120.28
2	B	273	ALA	C-N-CA	6.06	128.40	120.28
2	D	56	ALA	O-C-N	-6.06	115.79	122.09
2	D	298	ARG	CA-C-N	6.05	128.31	120.44
2	D	298	ARG	C-N-CA	6.05	128.31	120.44
1	A	604	LYS	CA-C-O	6.05	126.94	120.46
2	D	90	VAL	O-C-N	-6.05	116.07	123.09
2	D	483	PRO	N-CA-CB	6.05	108.57	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	LEU	O-C-N	-6.04	114.33	122.43
2	B	48	PRO	N-CA-CB	6.04	108.94	103.08
2	B	550	THR	CA-C-N	6.04	128.30	120.44
2	B	550	THR	C-N-CA	6.04	128.30	120.44
1	C	527	PRO	N-CA-CB	6.04	109.98	103.33
1	A	41	ALA	CA-C-O	6.04	126.81	119.38
1	C	426	GLU	CA-C-N	6.04	128.39	120.60
1	C	426	GLU	C-N-CA	6.04	128.39	120.60
1	C	534	LEU	O-C-N	-6.04	114.84	122.27
2	B	231	SER	CA-C-O	6.04	127.83	121.19
2	B	587	ALA	CA-C-O	-6.04	114.44	120.90
1	A	630	VAL	CA-C-O	-6.03	113.74	120.74
2	B	349	SER	CA-C-N	6.03	128.36	120.28
2	B	349	SER	C-N-CA	6.03	128.36	120.28
1	C	539	GLY	CA-C-O	6.03	126.96	120.75
2	D	617	LEU	N-CA-C	-6.03	99.36	109.07
1	C	264	VAL	CA-C-N	6.03	128.35	120.28
1	C	264	VAL	C-N-CA	6.03	128.35	120.28
1	A	362	SER	N-CA-CB	6.02	121.07	111.56
1	A	439	LYS	O-C-N	-6.02	114.16	122.46
1	A	573	GLU	CA-C-N	-6.02	114.92	123.10
1	A	573	GLU	C-N-CA	-6.02	114.92	123.10
1	C	64	TYR	N-CA-C	6.01	119.20	109.40
2	D	586	LYS	O-C-N	-6.01	115.87	122.07
2	D	147	PRO	N-CA-CB	6.01	109.88	103.39
2	D	536	HIS	CA-C-N	6.01	129.01	120.53
2	D	536	HIS	C-N-CA	6.01	129.01	120.53
1	C	688	ILE	CA-CB-CG1	6.01	120.61	110.40
2	D	239	ASN	CA-C-N	6.01	128.13	120.56
2	D	239	ASN	C-N-CA	6.01	128.13	120.56
2	B	413	ALA	CA-C-O	-6.01	114.69	121.00
2	D	407	SER	CA-C-N	6.00	128.33	120.28
2	D	407	SER	C-N-CA	6.00	128.33	120.28
2	D	432	ALA	CA-C-N	6.00	130.15	120.30
2	D	432	ALA	C-N-CA	6.00	130.15	120.30
1	A	272	SER	O-C-N	-6.00	114.45	122.43
1	C	391	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	C	69	PRO	CA-C-N	6.00	130.65	122.07
1	C	69	PRO	C-N-CA	6.00	130.65	122.07
1	A	504	ASP	CA-C-N	6.00	125.71	119.05
1	A	504	ASP	C-N-CA	6.00	125.71	119.05
1	A	665	VAL	CA-C-N	6.00	125.21	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	VAL	C-N-CA	6.00	125.21	118.97
1	C	23	ARG	NE-CZ-NH1	6.00	127.50	121.50
2	B	299	ALA	O-C-N	-6.00	115.76	122.12
2	B	550	THR	O-C-N	-6.00	115.76	122.12
1	C	181	THR	CA-C-N	5.99	128.56	120.65
1	C	181	THR	C-N-CA	5.99	128.56	120.65
1	A	66	GLY	O-C-N	-5.99	115.03	122.34
1	A	589	GLU	CA-C-N	5.99	128.23	120.44
1	A	589	GLU	C-N-CA	5.99	128.23	120.44
1	C	460	GLY	CA-C-N	5.99	128.30	120.28
1	C	460	GLY	C-N-CA	5.99	128.30	120.28
2	B	153	VAL	CA-C-N	5.98	132.41	122.54
2	B	153	VAL	C-N-CA	5.98	132.41	122.54
2	B	328	TRP	O-C-N	-5.98	115.33	122.15
2	B	263	VAL	N-CA-C	-5.98	104.91	110.53
1	C	282	PRO	O-C-N	-5.98	113.82	122.37
1	C	427	VAL	O-C-N	-5.98	115.96	121.94
1	C	497	VAL	O-C-N	-5.98	116.05	121.91
1	C	637	PRO	CA-C-N	5.98	128.78	120.29
1	C	637	PRO	C-N-CA	5.98	128.78	120.29
2	D	458	GLN	OE1-CD-NE2	5.98	128.58	122.60
2	B	117	ASP	CA-CB-CG	5.98	118.58	112.60
1	C	533	LYS	O-C-N	-5.98	115.91	122.07
1	C	573	GLU	O-C-N	-5.98	115.81	122.03
2	B	578	GLY	CA-C-O	5.98	130.97	120.57
1	C	600	ILE	N-CA-C	5.98	117.36	108.46
1	A	578	PRO	CA-C-N	5.97	128.77	120.29
1	A	578	PRO	C-N-CA	5.97	128.77	120.29
1	C	355	ALA	CA-C-O	5.97	127.29	120.90
2	D	328	TRP	O-C-N	-5.97	115.34	122.15
2	B	116	PRO	N-CA-CB	5.97	109.84	103.39
2	B	187	ASP	O-C-N	-5.97	114.65	122.59
1	C	703	GLU	CA-CB-CG	5.97	126.04	114.10
2	D	106	ALA	CA-C-N	-5.97	112.35	122.67
2	D	106	ALA	C-N-CA	-5.97	112.35	122.67
1	A	107	ALA	CA-C-N	5.96	132.82	122.56
1	A	107	ALA	C-N-CA	5.96	132.82	122.56
1	A	141	VAL	CA-CB-CG1	5.96	120.54	110.40
1	A	358	GLY	N-CA-C	-5.96	105.42	115.62
2	D	90	VAL	CA-CB-CG2	5.96	120.53	110.40
2	B	261	GLU	CA-C-N	5.96	129.37	120.31
2	B	261	GLU	C-N-CA	5.96	129.37	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	ARG	CA-C-N	5.96	128.86	120.28
1	C	697	ARG	C-N-CA	5.96	128.86	120.28
1	A	336	LEU	CA-C-O	5.96	127.77	120.92
1	A	524	ASP	O-C-N	-5.96	114.24	122.46
1	A	677	ARG	CD-NE-CZ	-5.96	116.06	124.40
2	B	243	ASN	O-C-N	-5.96	115.25	122.22
2	B	364	THR	O-C-N	-5.95	114.15	122.37
2	B	26	ASP	CA-C-O	5.95	126.69	119.31
1	C	469	LYS	CA-C-N	5.95	130.61	122.34
1	C	469	LYS	C-N-CA	5.95	130.61	122.34
1	A	256	MET	CB-CA-C	-5.94	101.55	110.88
1	C	215	GLN	CA-C-O	5.94	128.30	120.16
2	B	534	VAL	CB-CA-C	-5.94	104.36	111.97
2	B	576	GLN	CA-C-O	-5.94	114.58	120.70
2	D	495	GLU	CA-C-O	-5.94	114.22	120.63
1	A	230	ALA	CA-C-O	5.94	127.24	120.00
2	B	426	LEU	CA-C-N	5.94	130.72	122.29
2	B	426	LEU	C-N-CA	5.94	130.72	122.29
2	B	422	GLU	O-C-N	-5.93	115.96	122.07
2	B	169	ARG	NE-CZ-NH2	-5.93	113.87	119.20
1	A	428	GLU	CA-C-N	5.92	128.22	120.28
1	A	428	GLU	C-N-CA	5.92	128.22	120.28
1	C	153	PHE	O-C-N	-5.92	115.06	122.35
2	D	84	LYS	N-CA-C	-5.92	99.59	109.24
2	D	348	PHE	CA-C-N	5.92	128.49	120.38
2	D	348	PHE	C-N-CA	5.92	128.49	120.38
1	A	529	ARG	N-CA-CB	-5.91	101.74	110.49
2	D	347	THR	CA-C-O	5.91	127.03	120.82
1	A	25	PHE	CA-C-N	5.91	128.52	120.54
1	A	25	PHE	C-N-CA	5.91	128.52	120.54
1	A	379	SER	O-C-N	-5.91	115.41	122.15
2	B	449	ARG	CA-C-N	5.91	128.20	120.28
2	B	449	ARG	C-N-CA	5.91	128.20	120.28
1	C	385	ASN	N-CA-CB	5.91	119.31	110.22
1	C	397	THR	O-C-N	-5.91	114.37	122.46
1	C	686	GLY	N-CA-C	5.91	117.53	111.56
2	D	335	ASP	CA-C-N	5.90	125.52	119.56
2	D	335	ASP	C-N-CA	5.90	125.52	119.56
1	A	131	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	C	303	ALA	CA-C-O	5.90	126.81	120.55
2	D	435	THR	CA-C-N	5.90	131.46	122.37
2	D	435	THR	C-N-CA	5.90	131.46	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	157	VAL	CB-CA-C	-5.90	103.83	110.96
2	D	340	ILE	N-CA-C	-5.90	104.76	110.42
2	B	477	LYS	CA-C-O	5.89	126.21	119.61
2	D	229	PRO	N-CA-CB	5.89	108.95	103.41
1	A	541	ALA	CA-C-O	5.89	126.41	119.28
1	A	714	SER	CA-C-N	5.89	128.42	120.65
1	A	714	SER	C-N-CA	5.89	128.42	120.65
2	B	67	VAL	CA-C-N	5.89	132.26	122.66
2	B	67	VAL	C-N-CA	5.89	132.26	122.66
2	B	390	VAL	O-C-N	-5.89	115.23	122.18
1	C	488	VAL	CB-CA-C	-5.89	104.31	112.02
1	A	78	MET	O-C-N	-5.88	114.76	122.59
1	C	272	SER	O-C-N	-5.88	114.74	122.39
2	D	23	LEU	O-C-N	-5.88	114.77	122.59
2	D	393	GLY	CA-C-N	5.88	130.68	120.68
2	D	393	GLY	C-N-CA	5.88	130.68	120.68
2	B	200	ASP	CA-C-O	5.88	128.21	120.16
1	C	494	ALA	O-C-N	-5.87	115.89	122.12
2	D	288	HIS	CB-CG-CD2	5.87	138.84	131.20
2	B	233	ALA	CB-CA-C	-5.87	99.96	110.70
2	D	330	GLU	CA-C-O	-5.87	111.43	119.12
2	D	543	PRO	N-CA-CB	5.87	108.46	103.35
1	A	189	PRO	N-CA-CB	5.87	109.78	103.33
1	C	123	ARG	CA-C-N	5.86	131.74	120.66
1	C	123	ARG	C-N-CA	5.86	131.74	120.66
2	D	637	ALA	CA-C-N	5.86	132.25	121.70
2	D	637	ALA	C-N-CA	5.86	132.25	121.70
2	B	633	ILE	O-C-N	-5.86	116.19	121.87
2	D	537	ILE	O-C-N	-5.85	116.15	121.89
1	C	688	ILE	CA-C-O	5.85	127.79	119.95
1	A	695	GLU	CA-C-O	-5.85	114.35	120.55
2	B	435	THR	N-CA-CB	-5.85	100.61	110.49
1	C	505	PRO	N-CA-CB	5.85	109.70	103.39
1	A	648	ASP	CA-C-O	5.84	128.62	121.84
1	C	271	GLU	CA-C-N	5.84	129.95	120.60
1	C	271	GLU	C-N-CA	5.84	129.95	120.60
1	A	203	GLU	N-CA-CB	5.84	118.54	110.07
2	B	417	TRP	CA-C-N	5.84	128.03	120.44
2	B	417	TRP	C-N-CA	5.84	128.03	120.44
2	B	629	SER	O-C-N	-5.84	115.09	122.27
2	B	299	ALA	N-CA-CB	5.84	118.70	110.12
1	C	63	THR	N-CA-C	-5.83	101.56	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	MET	CA-C-N	5.83	130.56	120.58
1	A	149	MET	C-N-CA	5.83	130.56	120.58
1	A	307	LEU	CA-C-N	5.83	128.10	120.28
1	A	307	LEU	C-N-CA	5.83	128.10	120.28
1	A	332	SER	O-C-N	-5.83	115.61	122.96
1	A	598	PRO	N-CA-CB	5.83	108.52	103.27
2	D	331	LEU	CA-C-O	5.83	127.70	121.05
2	B	599	PHE	O-C-N	-5.83	115.40	122.22
1	C	655	SER	O-C-N	-5.83	115.42	123.12
2	D	410	ARG	N-CA-CB	5.83	118.42	109.91
2	D	490	TRP	O-C-N	-5.83	116.39	123.27
2	D	301	ARG	O-C-N	-5.83	115.84	122.08
2	D	586	LYS	CA-C-N	5.83	128.36	120.38
2	D	586	LYS	C-N-CA	5.83	128.36	120.38
1	A	573	GLU	CA-C-O	-5.83	114.66	121.07
1	A	677	ARG	N-CA-C	5.83	121.38	108.27
1	C	328	HIS	N-CA-C	-5.82	101.39	110.42
1	C	106	LEU	O-C-N	-5.82	115.51	122.15
1	C	367	SER	CA-C-N	5.82	128.88	120.38
1	C	367	SER	C-N-CA	5.82	128.88	120.38
2	B	95	ARG	CG-CD-NE	5.82	124.80	112.00
2	B	416	ALA	CA-C-N	5.82	128.00	120.44
2	B	416	ALA	C-N-CA	5.82	128.00	120.44
2	B	434	MET	O-C-N	-5.82	115.52	122.15
2	D	225	ALA	O-C-N	-5.82	115.42	122.22
2	B	141	ASP	O-C-N	-5.81	114.64	121.32
1	C	342	TYR	CA-C-N	5.81	128.65	120.28
1	C	342	TYR	C-N-CA	5.81	128.65	120.28
1	A	335	SER	O-C-N	-5.81	114.65	122.43
1	A	391	GLN	OE1-CD-NE2	-5.81	116.79	122.60
2	D	602	PHE	CA-C-N	5.81	130.06	120.25
2	D	602	PHE	C-N-CA	5.81	130.06	120.25
1	A	104	ARG	CA-C-N	5.80	127.98	120.44
1	A	104	ARG	C-N-CA	5.80	127.98	120.44
2	B	495	GLU	CA-C-N	5.80	128.41	120.46
2	B	495	GLU	C-N-CA	5.80	128.41	120.46
2	B	630	THR	N-CA-CB	5.80	118.75	110.16
1	C	25	PHE	N-CA-C	-5.80	104.87	111.14
1	A	500	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	C	622	ALA	O-C-N	-5.80	115.97	122.12
1	A	697	ARG	CD-NE-CZ	5.80	132.52	124.40
1	C	465	ILE	N-CA-C	5.80	116.76	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	585	GLU	O-C-N	-5.80	116.09	122.07
1	A	182	ALA	CA-C-N	5.80	128.32	120.38
1	A	182	ALA	C-N-CA	5.80	128.32	120.38
1	A	645	VAL	CA-C-N	5.80	131.77	120.99
1	A	645	VAL	C-N-CA	5.80	131.77	120.99
2	D	442	LEU	O-C-N	-5.80	116.10	122.07
2	B	154	LEU	CA-C-N	5.79	128.36	120.54
2	B	154	LEU	C-N-CA	5.79	128.36	120.54
1	A	232	MET	N-CA-CB	-5.79	102.69	111.21
1	A	321	LYS	CA-C-N	5.79	128.62	120.28
1	A	321	LYS	C-N-CA	5.79	128.62	120.28
2	B	503	ARG	CA-C-O	-5.79	114.41	120.55
1	C	136	VAL	CA-C-O	5.79	128.10	120.98
1	C	639	GLU	O-C-N	-5.79	115.84	122.09
2	D	268	GLU	CA-C-O	-5.79	114.74	120.82
1	C	205	MET	O-C-N	-5.79	115.55	122.15
1	A	155	GLY	O-C-N	-5.79	116.16	122.41
1	A	250	ALA	N-CA-C	5.79	118.62	110.23
1	A	385	ASN	CA-C-N	5.79	127.96	120.44
1	A	385	ASN	C-N-CA	5.79	127.96	120.44
1	C	323	MET	O-C-N	-5.78	114.39	122.37
1	C	671	GLU	CA-C-N	5.78	127.96	120.44
1	C	671	GLU	C-N-CA	5.78	127.96	120.44
2	B	456	ARG	CA-C-N	5.78	129.10	120.31
2	B	456	ARG	C-N-CA	5.78	129.10	120.31
1	A	202	LYS	CA-C-N	5.78	128.30	120.44
1	A	202	LYS	C-N-CA	5.78	128.30	120.44
2	B	149	HIS	CA-C-N	5.78	127.95	120.44
2	B	149	HIS	C-N-CA	5.78	127.95	120.44
1	C	295	PHE	CA-CB-CG	-5.78	108.02	113.80
1	C	423	HIS	O-C-N	-5.78	116.00	122.12
1	C	441	ILE	CA-C-N	5.78	125.25	119.24
1	C	441	ILE	C-N-CA	5.78	125.25	119.24
2	B	591	LYS	N-CA-CB	-5.78	101.33	110.28
1	A	80	ALA	CA-C-N	5.77	133.46	122.60
1	A	80	ALA	C-N-CA	5.77	133.46	122.60
1	C	532	LEU	CA-C-O	5.77	126.65	120.70
1	C	393	GLU	N-CA-C	5.77	120.98	113.88
2	B	543	PRO	N-CA-CB	5.77	108.37	103.35
1	C	248	ALA	O-C-N	-5.77	114.01	122.43
1	C	267	ILE	O-C-N	-5.77	115.90	121.90
2	B	252	LEU	CA-C-N	5.77	127.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	LEU	C-N-CA	5.77	127.94	120.44
2	B	480	PRO	N-CA-CB	5.77	108.44	103.31
2	D	267	VAL	N-CA-CB	5.77	118.38	110.54
1	C	115	VAL	N-CA-C	5.77	116.88	108.58
1	C	535	CYS	CA-C-O	5.77	126.53	120.42
2	B	340	ILE	CA-C-N	5.76	128.47	120.29
2	B	340	ILE	C-N-CA	5.76	128.47	120.29
1	A	426	GLU	CA-C-N	5.76	128.03	120.60
1	A	426	GLU	C-N-CA	5.76	128.03	120.60
2	D	310	VAL	O-C-N	-5.76	116.28	121.87
2	B	506	SER	CA-C-O	-5.76	114.31	120.42
1	C	689	PRO	N-CA-CB	5.76	108.44	103.31
1	A	411	GLU	CA-C-O	-5.76	114.77	120.82
2	B	401	GLY	O-C-N	-5.76	116.14	122.65
2	B	628	SER	O-C-N	-5.76	116.01	122.12
1	C	38	TRP	O-C-N	5.76	129.78	123.04
2	D	286	ALA	N-CA-C	-5.76	99.14	108.52
2	B	449	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	C	568	GLY	O-C-N	-5.75	114.70	122.35
1	A	229	SER	O-C-N	-5.75	115.49	122.22
1	C	677	ARG	O-C-N	-5.75	116.13	121.36
2	B	347	THR	O-C-N	-5.75	116.03	122.12
1	C	264	VAL	O-C-N	-5.75	116.19	121.94
2	B	32	GLU	O-C-N	-5.75	116.03	122.12
1	A	280	PHE	CA-C-N	5.74	129.47	120.97
1	A	280	PHE	C-N-CA	5.74	129.47	120.97
1	C	44	ILE	N-CA-CB	5.74	119.03	111.40
2	D	22	SER	N-CA-CB	5.74	119.58	110.57
1	A	585	GLU	CA-C-N	5.74	127.97	120.28
1	A	585	GLU	C-N-CA	5.74	127.97	120.28
2	B	636	VAL	N-CA-C	-5.74	100.15	108.87
2	D	78	PRO	CA-C-N	5.74	129.78	120.60
2	D	78	PRO	C-N-CA	5.74	129.78	120.60
1	C	401	ASP	CA-C-N	5.74	125.41	119.56
1	C	401	ASP	C-N-CA	5.74	125.41	119.56
2	B	408	LEU	CA-C-N	5.74	127.89	120.44
2	B	408	LEU	C-N-CA	5.74	127.89	120.44
1	C	127	SER	N-CA-C	5.74	119.54	112.54
2	D	329	ARG	NE-CZ-NH2	5.74	124.36	119.20
2	D	438	VAL	N-CA-CB	5.74	116.64	110.62
1	A	170	ALA	O-C-N	-5.73	112.36	121.53
1	A	352	ALA	O-C-N	-5.73	115.52	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	C	446	ILE	O-C-N	-5.73	115.93	121.83
2	D	397	ASP	CA-C-O	5.73	128.01	120.16
2	D	492	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	A	475	GLU	N-CA-CB	5.72	117.73	110.23
2	B	26	ASP	O-C-N	-5.72	114.56	122.46
1	A	265	ASP	O-C-N	-5.72	116.06	122.12
2	B	170	TYR	CA-C-O	-5.72	112.85	118.97
1	C	428	GLU	CA-C-N	5.72	127.95	120.28
1	C	428	GLU	C-N-CA	5.72	127.95	120.28
1	C	320	PRO	O-C-N	-5.72	114.84	122.22
1	A	381	ARG	NH1-CZ-NH2	-5.72	111.87	119.30
2	D	421	GLN	CA-C-N	5.72	128.26	120.54
2	D	421	GLN	C-N-CA	5.72	128.26	120.54
2	D	226	LYS	CA-C-N	5.71	131.79	121.06
2	D	226	LYS	C-N-CA	5.71	131.79	121.06
2	B	86	GLY	N-CA-C	-5.71	104.36	112.81
1	C	182	ALA	CA-C-N	5.71	128.25	120.54
1	C	182	ALA	C-N-CA	5.71	128.25	120.54
1	C	63	THR	O-C-N	-5.71	115.04	122.97
2	D	432	ALA	O-C-N	-5.71	116.16	122.09
2	B	33	GLU	CB-CG-CD	5.71	122.30	112.60
1	A	122	HIS	CB-CA-C	-5.70	101.33	110.79
2	B	289	ASP	CA-C-N	5.70	128.71	120.79
2	B	289	ASP	C-N-CA	5.70	128.71	120.79
1	C	537	ASP	CA-C-O	-5.70	114.38	120.42
1	C	667	ALA	CA-C-N	5.70	127.85	120.44
1	C	667	ALA	C-N-CA	5.70	127.85	120.44
1	C	387	GLN	CB-CG-CD	-5.69	102.92	112.60
1	A	44	ILE	N-CA-C	-5.69	101.24	107.73
1	A	145	SER	CA-C-N	5.69	129.46	120.47
1	A	145	SER	C-N-CA	5.69	129.46	120.47
1	C	383	ALA	O-C-N	-5.69	116.21	122.07
1	A	216	PRO	O-C-N	-5.69	114.88	122.22
1	C	169	GLY	O-C-N	-5.69	115.31	122.70
2	B	576	GLN	N-CA-C	5.68	117.28	111.14
1	C	500	ARG	NE-CZ-NH2	-5.68	114.08	119.20
2	D	245	GLY	CA-C-O	-5.68	112.78	118.86
2	D	299	ALA	CA-C-O	-5.68	114.85	120.82
1	A	477	PRO	N-CA-CB	5.68	108.36	103.31
1	A	586	LEU	O-C-N	-5.68	116.10	122.12
1	C	439	LYS	CA-C-O	5.68	126.38	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	553	ILE	O-C-N	-5.67	115.83	121.96
2	B	240	ILE	CA-C-O	-5.67	115.37	121.27
1	C	366	ASN	CA-CB-CG	-5.67	106.93	112.60
2	D	298	ARG	CD-NE-CZ	5.67	132.34	124.40
2	B	75	MET	CA-C-O	5.67	127.40	120.60
1	C	120	PRO	O-C-N	-5.67	116.06	122.18
1	C	231	ASN	N-CA-C	5.67	120.89	113.30
1	A	315	PHE	O-C-N	-5.66	114.16	122.43
2	B	420	PHE	O-C-N	-5.66	116.24	122.07
2	D	340	ILE	CA-C-N	5.66	128.13	120.44
2	D	340	ILE	C-N-CA	5.66	128.13	120.44
2	B	316	ASP	CA-C-N	5.66	131.70	122.65
2	B	316	ASP	C-N-CA	5.66	131.70	122.65
1	C	152	LEU	CB-CA-C	-5.66	101.76	110.81
1	A	218	MET	O-C-N	-5.65	116.13	122.12
1	A	344	ASN	O-C-N	-5.65	115.61	122.22
1	C	178	TYR	CA-C-N	5.65	128.21	120.46
1	C	178	TYR	C-N-CA	5.65	128.21	120.46
2	D	56	ALA	CA-C-N	5.65	128.13	120.44
2	D	56	ALA	C-N-CA	5.65	128.13	120.44
2	D	478	PRO	N-CA-CB	5.65	108.22	103.25
1	A	636	THR	CA-C-N	5.65	125.49	119.28
1	A	636	THR	C-N-CA	5.65	125.49	119.28
1	A	540	ARG	O-C-N	-5.64	115.33	122.27
2	D	82	PRO	N-CA-CB	5.64	108.26	103.35
2	D	216	VAL	CA-C-O	5.64	126.43	119.43
2	B	371	GLU	CA-CB-CG	5.64	125.37	114.10
1	A	147	TYR	CA-C-O	-5.63	114.87	120.90
2	D	548	GLY	N-CA-C	-5.63	104.15	111.52
2	D	108	ASP	N-CA-CB	-5.63	101.25	110.42
1	C	457	ILE	CA-C-N	5.62	127.82	120.28
1	C	457	ILE	C-N-CA	5.62	127.82	120.28
2	B	36	GLU	CA-C-N	5.62	127.81	120.28
2	B	36	GLU	C-N-CA	5.62	127.81	120.28
1	A	237	SER	N-CA-C	5.62	119.76	113.01
2	D	608	GLU	CA-C-N	5.62	128.13	120.54
2	D	608	GLU	C-N-CA	5.62	128.13	120.54
1	A	507	LYS	CA-C-N	5.62	127.72	120.70
1	A	507	LYS	C-N-CA	5.62	127.72	120.70
2	B	345	ILE	CA-C-N	5.62	128.08	120.44
2	B	345	ILE	C-N-CA	5.62	128.08	120.44
2	D	514	PHE	CA-C-O	-5.62	114.28	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	613	ILE	CA-C-O	5.62	126.58	120.57
1	A	86	ILE	N-CA-C	-5.62	100.59	108.12
1	C	43	GLN	O-C-N	-5.62	115.06	122.47
2	B	541	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	224	ILE	O-C-N	-5.61	116.05	121.83
1	A	422	GLY	O-C-N	-5.61	116.74	122.19
2	B	283	ARG	N-CA-C	-5.61	99.58	108.73
2	D	388	GLU	N-CA-C	5.61	119.30	112.23
2	B	242	HIS	O-C-N	-5.61	116.29	122.07
2	D	441	VAL	N-CA-C	-5.61	105.06	110.72
2	D	297	LEU	CA-C-N	5.61	130.16	120.58
2	D	297	LEU	C-N-CA	5.61	130.16	120.58
1	A	615	LYS	CA-C-O	-5.60	114.61	120.55
1	A	319	ASN	O-C-N	-5.60	115.14	121.36
1	C	661	HIS	N-CA-C	5.60	117.39	111.28
2	B	443	ASP	CB-CA-C	-5.60	101.33	110.85
1	C	42	GLU	CA-C-N	5.60	130.53	122.35
1	C	42	GLU	C-N-CA	5.60	130.53	122.35
1	C	674	LYS	O-C-N	-5.60	115.67	122.22
2	B	93	PHE	O-C-N	-5.60	116.00	121.87
1	C	280	PHE	CA-C-N	5.60	129.25	120.97
1	C	280	PHE	C-N-CA	5.60	129.25	120.97
1	A	339	GLN	CA-C-N	5.59	130.77	122.82
1	A	339	GLN	C-N-CA	5.59	130.77	122.82
1	A	454	GLN	O-C-N	-5.59	116.19	122.12
1	A	486	SER	CA-C-O	-5.59	114.59	120.63
1	A	589	GLU	O-C-N	-5.59	116.19	122.12
1	A	320	PRO	O-C-N	-5.59	115.01	122.22
2	B	27	PHE	CA-C-O	5.59	127.42	120.54
2	B	115	ASP	CA-C-N	5.59	125.43	119.28
2	B	115	ASP	C-N-CA	5.59	125.43	119.28
2	B	328	TRP	CA-C-O	5.59	126.34	120.42
1	A	451	ALA	CA-C-O	5.58	126.34	120.42
2	B	449	ARG	NH1-CZ-NH2	5.58	126.55	119.30
2	D	299	ALA	N-CA-CB	5.58	118.10	110.01
2	B	90	VAL	CA-C-N	5.58	128.60	120.51
2	B	90	VAL	C-N-CA	5.58	128.60	120.51
2	D	457	LYS	N-CA-C	-5.58	105.98	112.89
2	D	36	GLU	O-C-N	-5.57	116.21	122.12
1	C	298	VAL	O-C-N	-5.57	116.45	121.91
1	C	683	THR	O-C-N	-5.57	116.14	123.16
2	D	176	ALA	CA-C-N	5.57	127.68	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	176	ALA	C-N-CA	5.57	127.68	120.44
1	A	582	GLU	CA-C-N	5.57	128.00	120.65
1	A	582	GLU	C-N-CA	5.57	128.00	120.65
2	B	108	ASP	CB-CA-C	5.57	118.93	109.80
2	B	586	LYS	N-CA-C	-5.57	105.11	111.07
2	D	290	GLN	N-CA-C	5.57	117.03	111.07
2	D	309	GLU	CA-C-N	5.57	128.09	120.46
2	D	309	GLU	C-N-CA	5.57	128.09	120.46
1	C	655	SER	CA-C-O	5.57	126.24	120.40
2	D	305	ALA	CB-CA-C	-5.57	101.50	110.74
1	A	492	GLN	N-CA-C	-5.56	105.13	111.14
2	D	212	PRO	N-CA-CB	5.56	108.15	103.25
1	A	625	GLY	N-CA-C	5.56	122.15	114.92
1	C	663	THR	N-CA-C	-5.55	106.18	113.12
1	A	137	GLY	O-C-N	-5.55	115.98	122.31
1	A	236	ASN	N-CA-C	-5.55	100.13	108.96
2	B	212	PRO	N-CA-CB	5.55	108.25	103.31
2	B	294	ILE	O-C-N	-5.55	115.97	121.96
1	C	72	HIS	CB-CG-ND1	5.55	131.03	122.70
2	D	84	LYS	O-C-N	5.55	129.54	123.27
2	D	201	PRO	N-CA-CB	5.55	109.20	103.15
1	A	176	ALA	O-C-N	-5.55	116.24	122.12
1	A	24	ARG	CD-NE-CZ	5.55	132.16	124.40
1	A	380	ALA	O-C-N	-5.55	116.24	122.12
1	A	423	HIS	CA-C-N	5.55	128.06	120.46
1	A	423	HIS	C-N-CA	5.55	128.06	120.46
1	A	44	ILE	O-C-N	5.54	126.28	121.12
2	B	223	ARG	CA-C-N	5.54	132.42	122.38
2	B	223	ARG	C-N-CA	5.54	132.42	122.38
2	B	434	MET	CA-C-O	5.54	126.30	120.42
1	A	197	GLN	O-C-N	-5.54	116.27	122.03
1	C	16	PRO	N-CA-CB	5.54	108.49	103.34
1	C	130	PRO	N-CA-CB	5.54	109.57	103.26
2	B	137	LEU	N-CA-CB	5.54	119.89	110.87
2	B	416	ALA	CA-C-O	-5.54	114.55	120.42
2	D	187	ASP	CA-CB-CG	5.54	118.14	112.60
2	D	292	LEU	N-CA-C	-5.54	105.16	111.14
1	C	246	GLN	CA-C-N	5.53	128.25	120.28
1	C	246	GLN	C-N-CA	5.53	128.25	120.28
2	D	542	THR	O-C-N	-5.53	116.42	121.34
1	A	447	GLU	CA-C-O	5.53	126.41	120.55
2	D	223	ARG	CA-C-O	5.53	126.35	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	233	ALA	CA-C-O	5.53	126.38	120.24
2	B	342	ARG	CA-C-O	-5.53	114.69	120.55
2	D	272	THR	N-CA-C	-5.53	103.40	110.53
2	B	269	GLN	CB-CG-CD	5.53	121.99	112.60
2	D	200	ASP	CA-C-N	5.52	124.98	119.24
2	D	200	ASP	C-N-CA	5.52	124.98	119.24
1	C	155	GLY	O-C-N	-5.52	115.51	122.41
1	A	31	LYS	O-C-N	-5.52	116.27	122.12
2	D	115	ASP	CB-CG-OD1	5.52	131.09	118.40
1	C	419	LYS	CB-CA-C	5.52	119.54	110.88
1	C	18	PRO	N-CA-CB	5.51	108.57	103.39
1	A	222	SER	CA-C-N	5.51	130.05	120.68
1	A	222	SER	C-N-CA	5.51	130.05	120.68
2	B	25	GLY	CA-C-N	5.51	130.78	121.14
2	B	25	GLY	C-N-CA	5.51	130.78	121.14
1	A	64	TYR	N-CA-C	5.51	118.38	109.40
1	C	104	ARG	O-C-N	-5.51	116.40	122.07
2	D	350	ALA	CA-C-O	-5.51	114.58	120.42
2	D	188	LYS	CA-C-O	5.50	125.98	120.03
1	C	619	THR	O-C-N	-5.50	116.40	122.07
1	A	552	LEU	N-CA-C	-5.50	105.69	112.90
2	B	173	GLY	O-C-N	-5.50	116.90	122.18
1	A	309	ALA	CA-C-N	5.50	127.59	120.44
1	A	309	ALA	C-N-CA	5.50	127.59	120.44
2	B	510	ARG	CA-C-N	5.50	125.44	119.78
2	B	510	ARG	C-N-CA	5.50	125.44	119.78
2	D	347	THR	O-C-N	-5.50	116.41	122.07
2	D	627	LEU	CA-C-N	5.50	127.64	120.28
2	D	627	LEU	C-N-CA	5.50	127.64	120.28
2	B	388	GLU	N-CA-C	5.49	120.04	113.23
1	C	301	LEU	O-C-N	-5.49	116.30	122.12
2	D	280	ILE	N-CA-C	5.49	116.01	107.99
1	C	101	PHE	O-C-N	-5.49	116.42	122.07
1	C	554	LYS	CB-CA-C	-5.49	101.67	110.79
1	A	88	GLN	CA-C-N	5.49	128.63	120.95
1	A	88	GLN	C-N-CA	5.49	128.63	120.95
1	C	374	LEU	CA-C-O	5.49	126.68	120.70
2	D	189	PRO	N-CA-CB	5.49	109.01	103.25
1	C	360	THR	O-C-N	-5.48	116.54	122.79
2	B	58	CYS	CA-C-N	5.48	127.94	120.54
2	B	58	CYS	C-N-CA	5.48	127.94	120.54
2	B	141	ASP	CA-C-O	5.48	127.67	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ALA	O-C-N	-5.48	116.31	122.12
2	D	353	GLY	O-C-N	-5.48	115.57	122.70
2	D	364	THR	O-C-N	-5.48	114.28	122.39
1	A	17	VAL	N-CA-C	-5.48	101.63	107.77
2	D	425	LYS	O-C-N	-5.48	115.81	122.22
2	D	576	GLN	N-CA-C	5.48	117.11	111.03
1	C	8	ASP	N-CA-C	5.48	119.71	113.19
1	C	230	ALA	O-C-N	-5.48	115.11	122.23
2	D	66	THR	O-C-N	-5.47	116.22	122.68
1	C	262	ASP	CA-C-N	5.47	126.05	119.98
1	C	262	ASP	C-N-CA	5.47	126.05	119.98
1	A	235	TRP	CA-C-N	-5.47	114.91	122.30
1	A	235	TRP	C-N-CA	-5.47	114.91	122.30
1	C	206	VAL	CB-CA-C	-5.47	102.32	111.29
1	C	495	LYS	CA-C-N	5.47	128.06	120.29
1	C	495	LYS	C-N-CA	5.47	128.06	120.29
2	D	315	GLU	O-C-N	-5.47	115.28	122.39
1	A	560	THR	N-CA-C	-5.47	99.52	108.76
2	B	393	GLY	CA-C-N	5.47	130.71	121.14
2	B	393	GLY	C-N-CA	5.47	130.71	121.14
2	B	523	ASP	CA-C-O	-5.46	114.70	120.55
2	D	466	PHE	CB-CA-C	-5.46	107.32	111.20
1	A	66	GLY	CA-C-N	5.46	132.23	122.13
1	A	66	GLY	C-N-CA	5.46	132.23	122.13
1	A	93	SER	N-CA-CB	-5.46	101.26	110.49
2	B	100	ARG	O-C-N	5.46	129.49	123.16
2	B	520	THR	CA-C-N	5.46	127.60	120.28
2	B	520	THR	C-N-CA	5.46	127.60	120.28
1	A	515	ILE	O-C-N	-5.46	116.22	121.90
1	A	215	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	D	226	LYS	CB-CA-C	-5.46	102.25	110.92
1	A	130	PRO	N-CA-CB	5.45	109.09	103.15
1	A	445	ARG	O-C-N	-5.45	116.45	122.07
1	A	642	ARG	O-C-N	-5.45	116.45	122.07
2	B	88	PRO	O-C-N	-5.45	116.35	123.06
2	B	181	SER	CA-C-N	5.45	127.64	120.60
2	B	181	SER	C-N-CA	5.45	127.64	120.60
2	D	43	LEU	O-C-N	-5.45	115.56	122.27
1	A	502	GLU	CA-C-O	-5.45	113.36	119.79
2	B	189	PRO	CA-C-N	5.45	127.90	120.54
2	B	189	PRO	C-N-CA	5.45	127.90	120.54
2	D	341	LEU	CA-C-O	5.45	126.31	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	LEU	CA-C-N	5.45	131.69	122.65
1	C	368	LEU	C-N-CA	5.45	131.69	122.65
1	C	466	GLY	CA-C-O	5.45	125.17	119.07
2	D	141	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	492	GLN	CG-CD-NE2	5.45	124.57	116.40
1	C	131	ARG	O-C-N	-5.45	115.31	122.39
2	B	38	GLU	O-C-N	-5.44	116.35	122.12
2	B	128	GLY	O-C-N	-5.44	116.95	122.18
2	D	328	TRP	CA-C-O	5.44	126.19	120.42
1	A	54	VAL	CA-C-O	-5.44	114.60	120.47
1	C	421	TRP	CA-C-N	5.44	126.02	119.98
1	C	421	TRP	C-N-CA	5.44	126.02	119.98
2	D	529	GLY	CA-C-N	5.44	129.79	120.71
2	D	529	GLY	C-N-CA	5.44	129.79	120.71
1	A	142	ALA	O-C-N	-5.43	115.76	122.82
1	A	182	ALA	O-C-N	-5.43	116.47	122.07
1	C	233	PRO	N-CA-CB	5.43	108.91	103.48
2	B	77	ARG	NE-CZ-NH1	5.43	126.93	121.50
2	B	245	GLY	CA-C-N	-5.43	112.42	120.94
2	B	245	GLY	C-N-CA	-5.43	112.42	120.94
1	C	228	THR	N-CA-CB	5.43	117.94	110.07
1	C	509	LYS	CA-C-O	5.43	126.70	120.90
1	C	623	ASP	CA-C-N	5.43	132.79	121.94
1	C	623	ASP	C-N-CA	5.43	132.79	121.94
1	A	168	ASN	OD1-CG-ND2	-5.42	117.17	122.60
2	D	278	ASP	CA-C-O	-5.42	112.76	120.51
2	D	265	ALA	CA-C-O	-5.42	114.81	120.55
2	B	571	ALA	N-CA-CB	5.42	117.92	110.07
1	C	637	PRO	O-C-N	-5.42	115.23	122.22
2	D	34	GLN	N-CA-C	-5.42	105.29	111.14
1	A	110	GLN	N-CA-C	-5.41	102.87	110.50
1	A	352	ALA	CA-C-N	5.41	127.47	120.44
1	A	352	ALA	C-N-CA	5.41	127.47	120.44
1	A	470	TYR	CA-C-N	5.41	128.92	120.75
1	A	470	TYR	C-N-CA	5.41	128.92	120.75
1	A	304	ALA	O-C-N	-5.41	116.47	122.09
2	B	437	HIS	CA-C-O	-5.41	115.14	120.82
1	C	60	TRP	CA-C-N	5.41	129.33	120.63
1	C	60	TRP	C-N-CA	5.41	129.33	120.63
2	D	88	PRO	CB-CA-C	-5.41	102.90	110.63
2	D	204	PHE	O-C-N	-5.41	116.47	122.09
2	D	293	THR	O-C-N	-5.41	116.41	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LEU	O-C-N	-5.40	115.31	122.33
1	C	269	ALA	O-C-N	-5.40	116.50	122.07
1	C	402	PRO	N-CA-C	5.40	120.86	113.84
2	B	424	GLU	O-C-N	-5.40	116.51	122.07
1	A	514	LYS	CA-C-N	5.40	127.47	120.56
1	A	514	LYS	C-N-CA	5.40	127.47	120.56
2	B	329	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	D	211	GLU	CA-C-O	5.40	125.66	119.61
2	D	461	THR	O-C-N	-5.40	116.58	123.06
2	B	257	ALA	CA-C-N	5.39	127.95	120.29
2	B	257	ALA	C-N-CA	5.39	127.95	120.29
1	C	540	ARG	CA-C-N	5.39	131.84	122.56
1	C	540	ARG	C-N-CA	5.39	131.84	122.56
1	A	579	GLU	O-C-N	-5.39	116.00	122.15
2	D	60	LYS	CA-C-N	5.39	128.04	120.28
2	D	60	LYS	C-N-CA	5.39	128.04	120.28
2	B	322	GLN	CG-CD-NE2	5.39	124.48	116.40
1	C	600	ILE	O-C-N	-5.39	117.33	123.10
1	C	677	ARG	NH1-CZ-NH2	5.39	126.31	119.30
1	A	527	PRO	CA-C-N	5.39	129.22	120.60
1	A	527	PRO	C-N-CA	5.39	129.22	120.60
1	C	231	ASN	CB-CA-C	-5.39	101.07	110.17
1	A	72	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	A	465	ILE	CA-C-O	5.38	127.38	121.13
2	B	142	PRO	N-CA-CB	5.38	109.25	103.33
1	A	538	ALA	O-C-N	-5.38	116.02	122.15
1	C	664	LEU	N-CA-C	5.38	117.23	111.36
2	D	86	GLY	CA-C-N	5.38	135.38	122.36
2	D	86	GLY	C-N-CA	5.38	135.38	122.36
2	D	599	PHE	O-C-N	-5.38	115.92	122.22
1	C	244	HIS	CA-C-N	5.38	127.43	120.44
1	C	244	HIS	C-N-CA	5.38	127.43	120.44
2	B	448	GLU	N-CA-C	-5.38	105.33	111.14
1	A	137	GLY	CA-C-N	5.38	131.41	121.52
1	A	137	GLY	C-N-CA	5.38	131.41	121.52
1	A	273	VAL	N-CA-CB	5.37	119.42	112.28
1	A	530	ASN	OD1-CG-ND2	5.37	127.97	122.60
2	B	265	ALA	CA-C-O	-5.37	114.86	120.55
2	D	599	PHE	CA-C-N	5.37	128.01	120.28
2	D	599	PHE	C-N-CA	5.37	128.01	120.28
1	A	100	ALA	N-CA-C	-5.36	105.51	111.36
1	C	347	ARG	O-C-N	-5.36	116.51	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	31	THR	O-C-N	-5.36	116.97	123.03
2	D	193	LEU	N-CA-C	5.36	118.00	109.96
2	D	505	THR	O-C-N	-5.36	116.04	122.15
2	D	534	VAL	O-C-N	-5.36	116.66	121.91
2	B	366	ALA	N-CA-C	-5.36	106.74	113.28
1	C	245	MET	CA-C-O	-5.36	115.19	120.82
1	C	689	PRO	CA-C-N	5.36	128.20	120.38
1	C	689	PRO	C-N-CA	5.36	128.20	120.38
1	A	312	VAL	O-C-N	-5.35	116.68	121.87
2	B	397	ASP	O-C-N	-5.35	115.16	121.32
1	C	392	GLN	N-CA-C	5.35	119.89	112.45
2	D	291	PHE	CA-C-N	5.35	127.72	120.44
2	D	291	PHE	C-N-CA	5.35	127.72	120.44
1	C	302	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
2	D	378	ILE	O-C-N	-5.35	116.68	121.87
2	B	106	ALA	O-C-N	5.35	128.31	122.11
1	A	648	ASP	O-C-N	-5.35	115.92	122.55
1	C	403	TRP	CA-C-N	5.34	131.22	121.97
1	C	403	TRP	C-N-CA	5.34	131.22	121.97
2	B	22	SER	CA-C-O	5.34	126.58	120.54
2	B	496	VAL	CA-C-N	5.34	129.72	120.58
2	B	496	VAL	C-N-CA	5.34	129.72	120.58
2	B	27	PHE	CA-C-N	5.34	125.28	119.78
2	B	27	PHE	C-N-CA	5.34	125.28	119.78
1	A	51	ASN	O-C-N	-5.34	115.38	122.74
2	D	506	SER	CA-C-O	-5.34	114.07	120.10
1	A	141	VAL	N-CA-C	5.33	116.46	109.58
2	B	49	PRO	N-CA-CB	5.33	109.27	103.30
1	C	210	TYR	O-C-N	-5.33	116.71	122.79
1	C	604	LYS	CA-C-O	5.33	126.00	120.40
1	C	587	VAL	CA-C-N	5.33	127.37	120.44
1	C	587	VAL	C-N-CA	5.33	127.37	120.44
2	D	101	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	423	HIS	O-C-N	-5.33	116.47	122.12
2	B	39	VAL	CA-C-N	5.33	127.37	120.44
2	B	39	VAL	C-N-CA	5.33	127.37	120.44
2	B	365	GLN	O-C-N	-5.33	115.46	122.39
1	C	390	LEU	O-C-N	-5.33	116.47	122.12
1	C	520	GLY	CA-C-N	5.33	129.60	123.15
1	C	520	GLY	C-N-CA	5.33	129.60	123.15
2	D	229	PRO	CA-C-O	5.33	126.21	118.86
1	C	490	ALA	O-C-N	-5.33	116.47	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	216	VAL	O-C-N	-5.33	115.18	122.26
2	B	114	GLU	CA-CB-CG	5.32	124.75	114.10
2	D	114	GLU	CA-CB-CG	5.32	124.75	114.10
1	A	697	ARG	CA-C-N	5.32	128.40	120.31
1	A	697	ARG	C-N-CA	5.32	128.40	120.31
1	A	224	ILE	CA-C-N	5.32	127.67	120.65
1	A	224	ILE	C-N-CA	5.32	127.67	120.65
1	C	243	TYR	CA-C-N	5.32	127.41	120.28
1	C	243	TYR	C-N-CA	5.32	127.41	120.28
1	A	75	TYR	O-C-N	-5.32	116.46	123.21
2	D	33	GLU	CB-CG-CD	5.32	121.64	112.60
2	D	451	LYS	CA-C-N	5.32	127.84	120.29
2	D	451	LYS	C-N-CA	5.32	127.84	120.29
2	B	206	ALA	CA-C-O	-5.32	114.92	120.55
1	C	188	LYS	CA-C-N	5.32	125.38	119.32
1	C	188	LYS	C-N-CA	5.32	125.38	119.32
1	A	431	GLY	N-CA-C	5.31	122.65	115.32
1	C	140	GLY	CA-C-O	5.31	126.93	121.35
2	D	634	LEU	O-C-N	-5.31	113.91	122.41
1	A	129	ASN	CA-C-N	5.31	124.76	119.24
1	A	129	ASN	C-N-CA	5.31	124.76	119.24
1	A	263	GLY	O-C-N	-5.31	116.87	122.13
2	B	501	MET	CA-C-N	5.31	127.39	120.28
2	B	501	MET	C-N-CA	5.31	127.39	120.28
1	C	86	ILE	N-CA-C	-5.31	99.97	107.98
1	C	315	PHE	CA-C-N	5.31	130.20	121.87
1	C	315	PHE	C-N-CA	5.31	130.20	121.87
1	C	478	LEU	CA-C-O	5.31	125.86	120.24
1	C	256	MET	CA-CB-CG	5.30	124.71	114.10
2	D	500	LEU	N-CA-C	-5.30	105.58	111.36
2	B	524	PHE	CB-CG-CD1	5.30	129.71	120.70
2	D	206	ALA	CA-C-O	-5.30	114.93	120.55
2	B	195	LEU	CA-C-O	5.30	126.93	120.99
1	C	210	TYR	CA-C-N	5.30	131.51	121.97
1	C	210	TYR	C-N-CA	5.30	131.51	121.97
1	A	208	ASN	OD1-CG-ND2	5.30	127.90	122.60
2	B	167	PHE	CA-CB-CG	5.30	119.10	113.80
1	C	693	PHE	CA-CB-CG	5.30	119.10	113.80
2	B	224	LEU	CA-C-N	5.30	127.91	120.28
2	B	224	LEU	C-N-CA	5.30	127.91	120.28
2	D	268	GLU	N-CA-CB	5.30	117.69	110.01
2	B	573	VAL	CA-C-O	-5.29	115.44	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	130	GLU	CA-C-N	5.29	132.19	123.25
2	D	130	GLU	C-N-CA	5.29	132.19	123.25
2	D	559	LYS	O-C-N	-5.29	115.76	122.27
2	B	74	PRO	N-CA-CB	5.29	108.59	103.51
2	B	260	ALA	O-C-N	-5.29	116.62	122.07
1	C	72	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
2	B	425	LYS	O-C-N	-5.29	116.51	122.12
1	C	400	ILE	CA-C-N	5.29	134.71	121.80
1	C	400	ILE	C-N-CA	5.29	134.71	121.80
1	A	505	PRO	CA-C-N	5.29	127.32	120.44
1	A	505	PRO	C-N-CA	5.29	127.32	120.44
1	C	675	LEU	CA-C-N	5.29	129.55	121.51
1	C	675	LEU	C-N-CA	5.29	129.55	121.51
2	B	237	ASP	O-C-N	-5.29	115.97	122.68
1	C	357	GLN	CA-C-O	5.29	125.88	119.11
1	C	371	ALA	O-C-N	-5.28	113.91	122.42
1	A	578	PRO	O-C-N	-5.28	115.89	122.23
1	C	596	ARG	NE-CZ-NH1	5.28	126.78	121.50
2	B	462	ALA	O-C-N	-5.28	115.40	122.00
1	C	131	ARG	N-CA-C	5.28	118.82	112.38
1	C	400	ILE	O-C-N	-5.28	116.59	122.66
2	D	73	VAL	CA-C-N	5.28	126.44	119.84
2	D	73	VAL	C-N-CA	5.28	126.44	119.84
2	D	87	TYR	CA-C-N	5.28	125.73	120.14
2	D	87	TYR	C-N-CA	5.28	125.73	120.14
2	B	136	LEU	N-CA-C	5.28	118.08	109.59
1	C	59	ASP	CA-CB-CG	5.27	117.87	112.60
2	B	24	ALA	O-C-N	-5.27	115.79	122.27
2	D	556	ALA	N-CA-C	-5.27	105.43	111.07
1	A	282	PRO	N-CA-CB	5.27	108.75	103.48
1	A	696	LEU	N-CA-CB	5.27	117.86	110.12
2	B	626	THR	CA-C-O	-5.26	115.29	120.82
1	C	468	ASN	CA-CB-CG	5.26	117.86	112.60
2	B	310	VAL	O-C-N	-5.26	116.77	121.87
1	A	267	ILE	N-CA-C	-5.26	105.41	110.72
2	D	346	ALA	CA-C-O	-5.26	115.28	120.70
1	A	442	PRO	N-CA-CB	5.26	108.88	103.15
2	B	523	ASP	CB-CA-C	-5.26	101.96	110.79
1	C	42	GLU	O-C-N	-5.26	115.20	122.46
2	D	575	ALA	CA-C-O	-5.26	115.30	120.82
2	B	183	TYR	O-C-N	-5.25	116.55	122.12
2	B	315	GLU	CA-C-N	5.25	130.33	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	315	GLU	C-N-CA	5.25	130.33	121.14
1	C	311	LEU	CA-C-O	5.25	126.12	120.55
1	A	521	ASN	O-C-N	-5.25	116.64	121.42
2	B	201	PRO	N-CA-CB	5.25	109.11	103.33
2	B	63	THR	CA-CB-OG1	-5.25	101.73	109.60
1	C	311	LEU	CB-CA-C	-5.25	102.08	110.79
2	B	79	LYS	O-C-N	-5.25	115.57	122.39
1	C	184	GLU	N-CA-C	5.25	118.78	112.38
1	C	211	ILE	N-CA-CB	5.25	119.89	111.23
2	B	578	GLY	O-C-N	-5.25	115.88	122.70
2	D	383	GLY	O-C-N	-5.25	117.10	122.19
2	D	144	ALA	CA-C-O	-5.24	113.02	120.51
1	A	213	PRO	CA-C-N	5.24	126.39	119.84
1	A	213	PRO	C-N-CA	5.24	126.39	119.84
2	D	55	PHE	CA-CB-CG	-5.24	108.56	113.80
2	D	157	VAL	CA-C-O	5.24	126.78	120.65
1	A	16	PRO	N-CA-CB	5.24	108.21	103.34
2	D	192	ASP	N-CA-C	-5.23	105.25	111.69
1	A	522	PRO	N-CA-CB	5.23	108.21	103.34
1	C	53	ASP	CA-CB-CG	5.23	117.83	112.60
2	D	234	VAL	N-CA-C	5.23	115.50	108.17
1	A	400	ILE	CA-C-O	5.23	126.91	120.74
2	B	351	SER	N-CA-CB	5.23	117.59	110.01
2	B	292	LEU	CA-C-O	-5.23	114.88	120.42
1	C	300	LYS	CA-C-O	5.23	126.49	120.90
1	C	722	LEU	CA-C-N	5.23	127.23	120.44
1	C	722	LEU	C-N-CA	5.23	127.23	120.44
1	A	79	TYR	CA-C-N	5.22	127.80	120.28
1	A	79	TYR	C-N-CA	5.22	127.80	120.28
1	C	297	GLU	O-C-N	-5.22	116.58	122.12
2	D	58	CYS	CA-CB-SG	-5.22	102.39	114.40
2	D	200	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	548	MET	CA-C-O	-5.22	114.89	120.42
1	A	704	ILE	CA-C-O	5.22	125.82	120.39
2	B	380	ARG	CA-C-N	5.22	128.24	120.31
2	B	380	ARG	C-N-CA	5.22	128.24	120.31
2	B	407	SER	CA-C-N	5.22	127.28	120.28
2	B	407	SER	C-N-CA	5.22	127.28	120.28
2	B	445	CYS	O-C-N	-5.22	116.69	122.07
2	D	576	GLN	CA-C-O	-5.22	115.52	120.90
1	A	452	ARG	O-C-N	-5.22	116.69	122.07
1	C	667	ALA	O-C-N	-5.22	116.59	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLU	O-C-N	-5.22	116.59	122.12
1	A	59	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	363	PHE	CA-CB-CG	5.21	119.01	113.80
2	D	445	CYS	O-C-N	-5.21	116.61	122.03
2	D	268	GLU	CB-CA-C	-5.21	102.70	110.88
1	A	386	THR	O-C-N	-5.21	116.70	122.07
2	B	205	ALA	N-CA-CB	5.21	117.56	110.01
2	B	637	ALA	CA-C-N	5.21	131.07	121.70
2	B	637	ALA	C-N-CA	5.21	131.07	121.70
1	C	137	GLY	O-C-N	-5.21	116.38	122.31
1	C	305	ARG	CA-C-O	-5.21	115.03	120.55
2	D	374	PHE	CA-C-O	5.21	127.29	120.16
1	C	683	THR	N-CA-C	-5.20	101.68	109.95
2	B	240	ILE	N-CA-C	-5.20	104.90	110.36
1	A	459	SER	O-C-N	-5.20	115.46	122.43
2	B	90	VAL	CA-CB-CG2	5.20	119.24	110.40
2	B	389	GLU	CA-C-O	5.20	125.64	119.67
2	B	345	ILE	O-C-N	-5.19	116.48	121.83
1	C	381	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
1	A	638	GLU	O-C-N	-5.19	116.48	122.09
2	B	415	ALA	O-C-N	-5.19	116.72	122.07
2	B	544	GLN	OE1-CD-NE2	-5.19	117.41	122.60
2	D	266	LEU	CA-C-N	5.19	127.57	120.46
2	D	266	LEU	C-N-CA	5.19	127.57	120.46
1	C	281	ALA	CA-C-N	5.19	124.91	119.82
1	C	281	ALA	C-N-CA	5.19	124.91	119.82
1	A	253	ASP	CA-C-N	5.19	127.78	120.42
1	A	253	ASP	C-N-CA	5.19	127.78	120.42
2	D	408	LEU	CA-C-O	5.19	126.05	120.55
1	C	617	ILE	CA-C-O	-5.19	115.67	121.17
1	A	207	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	571	SER	CA-C-N	5.18	127.22	120.28
1	A	571	SER	C-N-CA	5.18	127.22	120.28
1	A	130	PRO	O-C-N	-5.18	116.59	122.18
1	A	342	TYR	CA-C-N	5.18	127.74	120.28
1	A	342	TYR	C-N-CA	5.18	127.74	120.28
2	B	513	VAL	N-CA-CB	5.18	118.86	111.82
2	B	490	TRP	O-C-N	-5.17	116.61	123.13
2	B	89	GLY	CA-C-O	5.17	124.76	119.02
1	C	582	GLU	CA-C-N	5.17	127.16	120.44
1	C	582	GLU	C-N-CA	5.17	127.16	120.44
2	D	259	GLY	N-CA-C	-5.17	106.23	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	TYR	CA-C-O	5.17	126.19	120.71
1	A	264	VAL	N-CA-C	-5.17	105.46	110.42
1	A	468	ASN	OD1-CG-ND2	-5.17	117.43	122.60
2	B	307	ILE	CA-C-O	-5.17	115.69	121.17
1	C	76	ALA	N-CA-C	5.17	117.31	111.11
1	A	105	ASN	CA-CB-CG	-5.16	107.44	112.60
2	B	167	PHE	N-CA-CB	5.16	120.28	111.66
1	C	4	LEU	N-CA-CB	5.16	119.56	110.37
1	C	80	ALA	O-C-N	-5.16	116.65	122.12
1	C	72	HIS	CG-CD2-NE2	5.16	112.36	107.20
1	C	512	LEU	O-C-N	-5.16	116.52	122.09
2	D	154	LEU	CA-C-N	5.16	127.50	120.54
2	D	154	LEU	C-N-CA	5.16	127.50	120.54
2	B	452	ARG	CA-C-N	5.16	127.46	120.44
2	B	452	ARG	C-N-CA	5.16	127.46	120.44
1	C	454	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	A	420	ALA	N-CA-CB	5.16	117.79	110.16
2	B	142	PRO	O-C-N	-5.16	116.04	122.23
1	C	354	ALA	O-C-N	-5.15	116.76	122.07
1	A	104	ARG	CG-CD-NE	5.15	123.34	112.00
1	C	25	PHE	N-CA-CB	5.15	117.54	110.07
1	A	345	VAL	N-CA-C	-5.15	105.69	110.53
2	B	261	GLU	O-C-N	-5.15	116.66	122.12
2	D	374	PHE	CA-C-N	5.15	124.46	118.85
2	D	374	PHE	C-N-CA	5.15	124.46	118.85
1	A	490	ALA	O-C-N	-5.15	116.73	122.09
2	B	400	GLY	CA-C-O	5.15	129.53	120.57
1	C	179	VAL	CA-C-N	5.15	127.73	120.42
1	C	179	VAL	C-N-CA	5.15	127.73	120.42
1	A	667	ALA	CA-C-O	-5.15	115.07	120.63
1	A	668	LEU	CA-C-N	5.15	127.13	120.44
1	A	668	LEU	C-N-CA	5.15	127.13	120.44
2	B	274	THR	O-C-N	-5.15	116.66	122.12
2	B	591	LYS	O-C-N	-5.15	115.94	122.27
1	C	452	ARG	O-C-N	-5.15	116.77	122.07
1	C	621	TYR	CA-C-N	5.15	127.18	120.28
1	C	621	TYR	C-N-CA	5.15	127.18	120.28
1	A	678	PRO	N-CA-CB	5.15	108.09	103.20
2	B	336	PRO	CA-C-N	5.15	127.69	120.28
2	B	336	PRO	C-N-CA	5.15	127.69	120.28
2	B	457	LYS	N-CA-C	-5.15	105.85	111.82
1	A	549	SER	CA-C-N	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	SER	C-N-CA	5.14	127.17	120.28
1	A	276	ASN	CA-C-O	-5.14	115.56	121.47
1	A	321	LYS	O-C-N	-5.14	116.20	122.22
1	A	510	ALA	CA-C-N	5.14	127.59	120.29
1	A	510	ALA	C-N-CA	5.14	127.59	120.29
1	C	26	GLU	CA-C-O	-5.14	115.40	120.90
1	C	122	HIS	CB-CA-C	-5.14	101.94	110.68
1	A	538	ALA	CA-C-O	5.14	125.87	120.42
2	B	452	ARG	CA-C-O	-5.14	114.06	119.97
1	A	703	GLU	O-C-N	-5.14	117.11	123.33
1	C	411	GLU	CA-C-N	5.14	127.17	120.28
1	C	411	GLU	C-N-CA	5.14	127.17	120.28
1	A	123	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	C	499	LEU	CA-C-N	5.13	127.16	120.28
1	C	499	LEU	C-N-CA	5.13	127.16	120.28
1	C	545	VAL	CA-C-N	5.13	125.64	119.94
1	C	545	VAL	C-N-CA	5.13	125.64	119.94
2	D	142	PRO	N-CA-CB	5.13	108.94	103.39
2	D	390	VAL	CA-C-O	5.13	125.17	119.42
2	D	131	ARG	N-CA-C	5.13	118.64	111.30
2	B	82	PRO	CA-C-N	5.13	127.11	120.44
2	B	82	PRO	C-N-CA	5.13	127.11	120.44
1	A	230	ALA	O-C-N	-5.13	114.74	122.28
1	A	63	THR	CA-C-N	5.13	130.63	122.94
1	A	63	THR	C-N-CA	5.13	130.63	122.94
1	A	198	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	191	GLN	OE1-CD-NE2	-5.12	117.47	122.60
1	C	493	LYS	O-C-N	-5.12	116.79	122.07
1	A	711	ILE	N-CA-C	5.12	119.94	108.88
1	C	326	ARG	CD-NE-CZ	5.12	131.57	124.40
2	B	176	ALA	O-C-N	-5.12	116.79	122.07
2	D	175	ALA	O-C-N	-5.12	116.69	122.12
1	A	562	GLN	O-C-N	-5.12	117.22	123.16
1	A	70	PHE	CB-CA-C	-5.12	104.33	111.80
1	A	215	GLN	N-CA-CB	5.12	119.48	110.37
2	D	482	ALA	CA-C-N	5.12	125.12	119.90
2	D	482	ALA	C-N-CA	5.12	125.12	119.90
1	A	669	ARG	CB-CG-CD	5.12	123.07	111.30
1	A	217	SER	N-CA-C	-5.12	105.70	111.28
2	D	137	LEU	N-CA-CB	5.12	118.88	110.90
2	D	497	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	469	LYS	CA-C-N	5.11	129.40	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LYS	C-N-CA	5.11	129.40	122.19
1	A	571	SER	O-C-N	-5.11	116.70	122.12
2	B	247	GLY	N-CA-C	-5.11	103.55	112.55
1	C	651	VAL	N-CA-C	5.11	115.10	108.35
2	D	523	ASP	CB-CA-C	-5.11	102.20	110.79
2	B	632	ASP	CA-C-N	5.11	127.46	120.46
2	B	632	ASP	C-N-CA	5.11	127.46	120.46
1	C	578	PRO	CA-C-N	5.11	127.08	120.44
1	C	578	PRO	C-N-CA	5.11	127.08	120.44
2	D	39	VAL	CA-C-O	-5.11	115.75	121.17
1	A	353	MET	O-C-N	-5.11	116.81	122.07
2	D	32	GLU	O-C-N	-5.11	116.70	122.12
1	A	499	LEU	CA-C-N	5.11	127.12	120.28
1	A	499	LEU	C-N-CA	5.11	127.12	120.28
2	B	461	THR	O-C-N	-5.11	116.93	123.06
1	C	538	ALA	CA-C-N	5.11	125.65	119.98
1	C	538	ALA	C-N-CA	5.11	125.65	119.98
2	D	370	PRO	N-CA-CB	5.10	107.79	103.35
1	A	7	PHE	N-CA-C	5.10	119.49	113.16
1	C	289	GLY	N-CA-C	-5.10	103.41	112.54
1	C	712	PRO	N-CA-CB	5.10	108.94	103.33
2	D	308	GLY	O-C-N	-5.10	116.07	122.70
2	D	557	PHE	O-C-N	-5.10	116.79	122.09
2	B	130	GLU	O-C-N	-5.09	114.99	122.43
2	B	613	ILE	N-CA-C	5.09	116.03	108.23
2	D	257	ALA	CA-C-N	5.09	128.05	120.31
2	D	257	ALA	C-N-CA	5.09	128.05	120.31
2	D	286	ALA	CA-C-N	-5.09	112.76	123.20
2	D	286	ALA	C-N-CA	-5.09	112.76	123.20
2	B	318	ARG	CD-NE-CZ	5.09	131.53	124.40
1	C	129	ASN	N-CA-C	-5.09	101.89	109.42
1	A	645	VAL	N-CA-CB	5.09	116.50	110.55
2	B	162	THR	N-CA-C	5.09	117.36	108.76
2	B	258	THR	CA-C-N	5.09	125.59	119.94
2	B	258	THR	C-N-CA	5.09	125.59	119.94
2	B	421	GLN	O-C-N	-5.09	116.83	122.07
2	B	520	THR	O-C-N	-5.09	116.94	122.84
1	C	331	THR	N-CA-C	-5.09	103.43	110.35
1	C	353	MET	N-CA-C	-5.09	105.82	111.36
2	D	253	ALA	N-CA-CB	5.09	117.52	109.94
2	B	30	ALA	O-C-N	-5.08	116.69	122.89
1	A	134	GLY	O-C-N	-5.08	116.95	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ILE	N-CA-C	-5.08	105.75	110.53
2	B	427	GLY	CA-C-O	-5.08	113.87	118.95
2	B	147	PRO	N-CA-CB	5.08	109.05	103.26
1	A	89	TYR	CA-C-O	-5.08	114.97	120.81
2	B	34	GLN	O-C-N	-5.08	116.84	122.07
1	A	131	ARG	O-C-N	-5.08	116.41	122.20
2	B	612	LEU	CA-C-O	5.08	125.21	119.27
1	C	31	LYS	CA-C-O	5.08	125.93	120.55
1	A	216	PRO	CA-C-N	5.07	127.08	120.28
1	A	216	PRO	C-N-CA	5.07	127.08	120.28
2	B	315	GLU	N-CA-C	5.07	117.47	111.33
1	C	99	ASN	OD1-CG-ND2	5.07	127.67	122.60
2	D	402	SER	N-CA-C	-5.07	102.79	110.24
1	A	252	ALA	N-CA-C	5.07	117.19	111.11
1	A	392	GLN	OE1-CD-NE2	-5.07	117.53	122.60
2	B	413	ALA	N-CA-C	-5.07	105.45	110.97
2	B	464	SER	N-CA-CB	5.07	118.10	110.65
2	D	214	LEU	N-CA-C	5.07	119.10	113.02
1	A	385	ASN	O-C-N	-5.07	116.04	122.27
1	A	413	THR	CA-C-N	5.07	127.03	120.44
1	A	413	THR	C-N-CA	5.07	127.03	120.44
1	A	689	PRO	CA-C-N	5.07	127.57	120.28
1	A	689	PRO	C-N-CA	5.07	127.57	120.28
2	D	40	GLU	N-CA-C	5.07	116.80	111.28
2	D	408	LEU	N-CA-C	5.07	116.80	111.28
1	A	222	SER	O-C-N	-5.06	116.30	122.22
2	D	543	PRO	N-CA-C	-5.06	103.16	111.21
1	A	550	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	556	ALA	N-CA-C	-5.06	105.65	111.07
1	C	367	SER	O-C-N	-5.06	116.78	123.16
1	A	123	ARG	CA-C-N	5.06	130.23	120.66
1	A	123	ARG	C-N-CA	5.06	130.23	120.66
2	D	191	LYS	N-CA-C	5.06	118.94	112.87
1	A	527	PRO	O-C-N	-5.06	116.16	122.23
2	B	423	VAL	O-C-N	-5.06	116.95	121.91
2	B	444	ALA	CA-C-N	5.06	127.01	120.44
2	B	444	ALA	C-N-CA	5.06	127.01	120.44
1	C	39	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	44	ILE	O-C-N	5.05	125.57	120.92
1	C	369	ASP	CB-CG-OD2	5.05	130.02	118.40
1	A	703	GLU	CA-C-N	5.05	129.82	123.10
1	A	703	GLU	C-N-CA	5.05	129.82	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	140	VAL	O-C-N	-5.05	116.26	122.88
1	C	263	GLY	O-C-N	-5.05	117.34	122.19
1	A	143	ILE	N-CA-CB	5.05	118.20	111.64
2	B	314	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	563	ILE	CB-CA-C	-5.05	104.65	110.91
2	B	105	ASP	CA-C-N	5.04	129.05	120.88
2	B	105	ASP	C-N-CA	5.04	129.05	120.88
2	B	608	GLU	CA-C-N	5.04	127.35	120.54
2	B	608	GLU	C-N-CA	5.04	127.35	120.54
1	C	251	THR	CA-C-N	5.04	127.04	120.28
1	C	251	THR	C-N-CA	5.04	127.04	120.28
2	D	413	ALA	O-C-N	-5.04	116.78	122.03
1	A	587	VAL	CA-C-N	5.04	127.00	120.44
1	A	587	VAL	C-N-CA	5.04	127.00	120.44
1	C	77	THR	OG1-CB-CG2	-5.04	99.22	109.30
2	D	396	ASN	CB-CG-ND2	-5.04	108.84	116.40
1	A	617	ILE	N-CA-C	-5.04	105.48	110.62
2	D	291	PHE	CB-CA-C	5.04	120.34	110.67
1	A	684	VAL	CA-C-O	5.04	125.70	120.36
1	C	626	PHE	CA-C-O	-5.04	115.87	121.81
2	D	439	THR	CA-C-N	5.04	127.97	120.31
2	D	439	THR	C-N-CA	5.04	127.97	120.31
1	A	295	PHE	O-C-N	-5.04	116.41	122.15
2	B	21	LEU	O-C-N	-5.04	116.62	122.96
1	C	213	PRO	CA-C-N	5.04	126.14	119.84
1	C	213	PRO	C-N-CA	5.04	126.14	119.84
1	C	302	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	A	442	PRO	CA-N-CD	-5.03	104.96	112.00
1	A	471	ARG	CD-NE-CZ	5.03	131.44	124.40
1	A	52	GLU	CA-C-N	5.03	127.52	120.28
1	A	52	GLU	C-N-CA	5.03	127.52	120.28
1	A	301	LEU	CA-C-O	-5.03	115.22	120.55
2	B	634	LEU	CA-C-N	5.03	131.26	121.41
2	B	634	LEU	C-N-CA	5.03	131.26	121.41
1	C	714	SER	CA-C-N	5.03	126.98	120.44
1	C	714	SER	C-N-CA	5.03	126.98	120.44
2	D	97	THR	CA-CB-OG1	-5.03	102.06	109.60
2	D	613	ILE	N-CA-C	5.03	115.55	108.36
2	B	45	ARG	N-CA-CB	5.03	117.52	109.28
1	C	598	PRO	N-CA-CB	5.03	107.78	103.36
1	C	633	LEU	N-CA-C	-5.03	104.23	110.41
2	B	441	VAL	N-CA-C	-5.02	105.81	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	638	GLU	O-C-N	-5.02	116.42	122.15
2	B	420	PHE	CA-C-N	5.02	126.97	120.44
2	B	420	PHE	C-N-CA	5.02	126.97	120.44
1	C	689	PRO	O-C-N	-5.02	116.95	123.03
2	D	348	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	74	PRO	O-C-N	-5.02	115.50	122.27
2	D	139	ARG	CA-C-N	-5.02	116.28	123.11
2	D	139	ARG	C-N-CA	-5.02	116.28	123.11
1	A	155	GLY	CA-C-O	5.02	125.84	119.72
1	C	21	ALA	CA-C-O	5.02	126.59	121.07
1	C	132	VAL	N-CA-C	5.02	117.72	112.90
2	D	376	LEU	CA-C-N	5.02	126.96	120.44
2	D	376	LEU	C-N-CA	5.02	126.96	120.44
2	B	522	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	C	438	GLU	CA-C-N	5.01	131.35	121.58
1	C	438	GLU	C-N-CA	5.01	131.35	121.58
1	A	643	GLN	N-CA-CB	5.01	117.57	110.16
1	C	452	ARG	CA-C-O	5.01	126.08	120.82
2	D	374	PHE	O-C-N	-5.01	115.56	121.32
1	C	109	GLY	N-CA-C	5.00	122.20	115.00
2	D	30	ALA	CA-C-O	5.00	126.39	120.69
2	D	494	SER	CA-C-N	5.00	127.23	120.38
2	D	494	SER	C-N-CA	5.00	127.23	120.38
1	A	320	PRO	N-CA-CB	5.00	108.79	103.39
1	C	88	GLN	CB-CG-CD	-5.00	104.10	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	GLY	Mainchain
1	C	167	MET	Mainchain
2	D	456	ARG	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5601	0	5540	44	0
1	C	5601	0	5540	41	0
2	B	4731	0	4667	33	0
2	D	4731	0	4667	46	0
3	A	54	0	37	1	0
3	C	54	0	37	1	0
4	A	91	0	88	12	0
4	C	91	0	88	8	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
6	A	356	0	0	0	0
6	B	219	0	0	0	0
6	C	361	0	0	1	0
6	D	214	0	0	0	0
All	All	22116	0	20680	173	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 4.

All (173) 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)
4:A:1800:B12:H531	4:A:1800:B12:H552	1.23	1.14
1:A:638:GLU:HA	1:A:671:GLU:HG2	1.58	0.86
1:A:635:GLN:HE22	1:A:643:GLN:HE21	1.28	0.79
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.67	0.77
1:C:635:GLN:HE22	1:C:643:GLN:HE21	1.35	0.74
4:A:1800:B12:H362	4:A:1800:B12:H351	1.70	0.74
4:C:2800:B12:H552	4:C:2800:B12:H531	1.71	0.72
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.71	0.72
1:A:650:HIS:HB3	1:A:722:LEU:HD11	1.74	0.70
2:B:468:MET:HE2	2:B:471:ALA:HA	1.74	0.68
2:D:180:VAL:HG13	2:D:197:LEU:HD21	1.74	0.68
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.76	0.68
1:A:706:THR:HB	1:A:707:PRO:HD2	1.75	0.68
1:A:247:GLU:HB3	4:A:1800:B12:H532	1.76	0.67
4:C:2800:B12:H351	4:C:2800:B12:H362	1.76	0.67
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.77	0.66
2:D:308:GLY:HA3	2:D:318:ARG:HG2	1.77	0.66
2:B:617:LEU:HD22	2:B:621:MET:HE1	1.77	0.66
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.76	0.66
1:A:14:ASN:HA	2:B:410:ARG:HH22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:GLU:HA	1:C:671:GLU:HG2	1.78	0.65
2:D:532:SER:HB3	2:D:533:PRO:HD3	1.80	0.64
2:D:370:PRO:HB3	2:D:375:PRO:HG2	1.80	0.64
1:C:706:THR:HB	1:C:707:PRO:CD	2.30	0.62
2:D:80:ASP:HB3	2:D:407:SER:HB2	1.81	0.62
4:A:1800:B12:H531	4:A:1800:B12:C55	2.10	0.62
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.81	0.61
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.83	0.61
2:D:138:LEU:HD23	2:D:145:ILE:HD13	1.83	0.61
1:A:359:HIS:CE1	1:A:401:ASP:H	2.18	0.60
1:C:706:THR:HB	1:C:707:PRO:HD2	1.82	0.60
4:C:2800:B12:C61	4:C:2800:B12:H551	2.33	0.59
1:A:706:THR:HB	1:A:707:PRO:CD	2.32	0.59
1:C:359:HIS:CE1	1:C:401:ASP:H	2.20	0.59
1:A:605:MET:HE3	1:A:664:LEU:HB3	1.85	0.57
2:B:565:ALA:HB3	2:B:593:LEU:HD23	1.88	0.56
1:A:4:LEU:HD13	2:B:264:ARG:HG2	1.86	0.56
2:D:141:ASP:HB3	2:D:142:PRO:HD2	1.86	0.56
2:B:503:ARG:HD2	2:B:638:LYS:HD3	1.88	0.56
1:C:247:GLU:HB3	4:C:2800:B12:H532	1.86	0.56
1:A:14:ASN:HA	2:B:410:ARG:NH2	2.21	0.55
4:A:1800:B12:H353	4:A:1800:B12:H302	1.89	0.55
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.88	0.55
4:C:2800:B12:H531	4:C:2800:B12:C55	2.36	0.55
1:C:139:ALA:HB1	4:C:2800:B12:H362	1.89	0.55
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.89	0.55
2:D:386:LEU:HD23	2:D:390:VAL:HG21	1.88	0.54
1:A:635:GLN:HE22	1:A:643:GLN:NE2	2.01	0.54
2:D:435:THR:HG22	2:D:436:GLU:H	1.72	0.54
1:A:635:GLN:NE2	1:A:643:GLN:HE21	2.03	0.54
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.91	0.53
4:C:2800:B12:H351	4:C:2800:B12:H372	1.90	0.53
2:D:201:PRO:HG3	2:D:217:LEU:HD21	1.90	0.53
2:D:429:MET:HE3	2:D:433:VAL:HG23	1.91	0.53
4:A:1800:B12:H362	4:A:1800:B12:C35	2.39	0.53
2:B:563:GLN:HE21	2:B:591:LYS:HD3	1.73	0.53
4:A:1800:B12:H552	4:A:1800:B12:C53	2.14	0.53
1:C:14:ASN:HA	2:D:410:ARG:NH2	2.24	0.52
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.92	0.52
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.40	0.52
2:D:281:ASN:ND2	2:D:323:ASN:HD21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:369:LEU:HB2	2:D:477:LYS:HG3	1.92	0.52
1:C:571:SER:HB3	1:C:623:ASP:HB3	1.91	0.52
4:A:1800:B12:H351	4:A:1800:B12:H372	1.91	0.52
2:B:431:LYS:HE2	2:B:434:MET:HE3	1.91	0.51
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.58	0.51
1:A:200:ILE:HG12	1:A:217:SER:HB3	1.93	0.51
1:C:252:ALA:O	1:C:256:MET:HG3	2.11	0.51
1:A:652:VAL:HG11	1:A:668:LEU:HD11	1.91	0.51
2:D:564:VAL:HG22	2:D:592:ALA:HB3	1.91	0.51
1:A:359:HIS:HE1	1:A:401:ASP:H	1.59	0.51
2:D:554:VAL:HG21	2:D:584:ALA:HB1	1.93	0.51
2:D:158:LEU:HD12	2:D:161:MET:SD	2.51	0.50
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.92	0.50
1:A:372:ILE:HG22	1:A:480:VAL:HG11	1.93	0.50
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.46	0.50
1:A:512:LEU:HD21	1:A:543:ALA:HB1	1.94	0.50
1:C:577:THR:HG22	1:C:580:VAL:H	1.77	0.50
1:C:7:PHE:HA	1:C:10:VAL:HG23	1.95	0.49
1:C:635:GLN:HE22	1:C:643:GLN:NE2	2.05	0.49
1:A:139:ALA:HB1	4:A:1800:B12:H362	1.95	0.49
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.95	0.48
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.78	0.48
2:D:284:VAL:HG21	2:D:297:LEU:HD22	1.95	0.48
1:A:666:PRO:O	1:A:670:LYS:HD2	2.12	0.48
2:B:429:MET:HE3	2:B:433:VAL:HG23	1.94	0.48
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.96	0.48
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.41	0.47
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.97	0.47
1:C:359:HIS:HE1	1:C:401:ASP:H	1.61	0.47
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.96	0.47
1:A:606:GLY:O	1:A:634:PHE:HA	2.15	0.47
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.78	0.47
2:B:579:LEU:HG	2:B:583:LYS:HD2	1.97	0.47
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.45	0.47
1:C:563:ILE:HD11	6:C:3184:HOH:O	2.15	0.47
2:D:325:ILE:HD11	2:D:361:LEU:HD21	1.96	0.47
1:A:597:ARG:HB3	1:A:598:PRO:HD2	1.96	0.46
1:A:691:GLN:NE2	1:A:691:GLN:H	2.14	0.46
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.96	0.46
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.97	0.46
1:C:691:GLN:HE21	1:C:691:GLN:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.98	0.46
1:C:691:GLN:H	1:C:691:GLN:NE2	2.13	0.46
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.98	0.46
2:D:191:LYS:HD2	2:D:226:LYS:O	2.15	0.46
1:A:635:GLN:NE2	1:A:643:GLN:NE2	2.63	0.46
1:C:392:GLN:HB3	2:D:459:PRO:HG2	1.97	0.46
1:A:36:GLU:H	1:A:36:GLU:CD	2.24	0.46
2:D:258:THR:OG1	2:D:429:MET:HG2	2.16	0.46
1:C:452:ARG:HA	1:C:573:GLU:HG2	1.98	0.46
4:A:1800:B12:H351	4:A:1800:B12:C36	2.38	0.45
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.51	0.45
2:D:390:VAL:HG12	2:D:392:ILE:HG23	1.98	0.45
1:C:571:SER:HB2	1:C:584:ARG:HH22	1.81	0.45
2:B:158:LEU:HD12	2:B:161:MET:SD	2.56	0.45
1:C:287:PHE:CE2	3:C:2801:3CP:HP11	2.52	0.45
1:A:571:SER:HB3	1:A:623:ASP:HB3	1.97	0.45
1:A:10:VAL:HG11	2:B:310:VAL:HG21	1.97	0.45
1:A:521:ASN:O	1:A:529:ARG:HD3	2.16	0.45
1:A:218:MET:HE1	1:A:266:TYR:CD2	2.52	0.45
2:B:554:VAL:HG21	2:B:584:ALA:HB1	1.99	0.45
1:A:20:ASP:OD2	1:A:24:ARG:HD2	2.16	0.44
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.98	0.44
1:C:599:ARG:HG2	1:C:649:VAL:HA	1.99	0.44
2:D:571:ALA:HA	2:D:601:GLU:HB3	2.00	0.44
2:D:503:ARG:HD2	2:D:638:LYS:HD3	1.99	0.44
1:A:691:GLN:H	1:A:691:GLN:HE21	1.65	0.44
2:B:334:GLU:O	2:B:335:ASP:C	2.60	0.44
1:A:319:ASN:HA	1:A:320:PRO:HD2	1.86	0.44
2:D:118:GLU:HG3	2:D:152:GLU:OE1	2.18	0.44
3:A:1801:3CP:OP2	3:A:1801:3CP:HB1	2.17	0.44
2:D:347:THR:O	2:D:348:PHE:C	2.59	0.44
1:A:372:ILE:HD13	1:A:478:LEU:HD23	1.99	0.43
1:C:317:PRO:HG2	1:C:323:MET:HE2	2.00	0.43
2:D:274:THR:HG23	2:D:317:LYS:HD3	1.99	0.43
2:D:284:VAL:HG11	2:D:322:GLN:HE21	1.83	0.43
1:A:686:GLY:O	1:A:707:PRO:HD3	2.18	0.43
1:A:252:ALA:O	1:A:256:MET:HG3	2.18	0.43
2:B:238:ALA:HB1	2:B:251:GLU:HG3	2.01	0.43
2:D:334:GLU:O	2:D:335:ASP:C	2.61	0.43
1:A:138:MET:SD	1:A:485:ASN:HB2	2.59	0.43
4:C:2800:B12:H362	4:C:2800:B12:C35	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:GLY:O	1:C:634:PHE:HA	2.19	0.43
2:D:169:ARG:HG2	2:D:207:LEU:HD13	2.01	0.43
1:C:14:ASN:O	1:C:15:ALA:C	2.62	0.43
1:C:521:ASN:O	1:C:529:ARG:HD3	2.19	0.42
1:A:641:ALA:O	1:A:645:VAL:HG23	2.19	0.42
1:C:319:ASN:HA	1:C:320:PRO:HD2	1.83	0.42
1:C:635:GLN:NE2	1:C:643:GLN:HE21	2.10	0.42
2:D:617:LEU:HD22	2:D:621:MET:HE1	2.00	0.42
1:A:54:VAL:O	1:A:58:MET:HE3	2.19	0.42
2:B:313:VAL:O	2:B:314:ASP:C	2.62	0.42
1:A:683:THR:HG21	1:A:718:LEU:HD13	2.02	0.42
2:D:532:SER:CB	2:D:533:PRO:HD3	2.49	0.42
2:B:347:THR:HG23	2:B:358:ILE:HG21	2.01	0.42
1:A:721:LYS:HA	1:A:721:LYS:HD3	1.95	0.41
4:A:1800:B12:H351	4:A:1800:B12:C37	2.49	0.41
2:B:242:HIS:CD2	2:B:285:THR:HG21	2.55	0.41
4:A:1800:B12:C35	4:A:1800:B12:H372	2.51	0.41
1:C:36:GLU:CD	1:C:36:GLU:H	2.27	0.41
2:B:252:LEU:HD11	2:B:300:LEU:HA	2.02	0.41
2:D:217:LEU:O	2:D:221:VAL:HG23	2.21	0.41
2:D:141:ASP:HB3	2:D:142:PRO:CD	2.51	0.41
2:D:234:VAL:HB	2:D:280:ILE:HA	2.03	0.41
2:D:267:VAL:HA	2:D:271:PHE:O	2.21	0.41
1:C:65:ALA:HA	1:C:72:HIS:HB2	2.03	0.41
1:C:207:ARG:HD2	1:C:244:HIS:CD2	2.56	0.41
2:B:83:LYS:HE3	2:B:83:LYS:HA	2.03	0.40
2:B:331:LEU:HD13	2:B:365:GLN:HB3	2.04	0.40
1:C:372:ILE:HG22	1:C:480:VAL:HG11	2.03	0.40
1:A:261:ALA:O	1:A:262:ASP:C	2.64	0.40
1:C:89:TYR:HA	1:C:114:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/727 (100%)	695 (96%)	30 (4%)	0	100	100
1	C	725/727 (100%)	694 (96%)	31 (4%)	0	100	100
2	B	617/637 (97%)	601 (97%)	15 (2%)	1 (0%)	43	51
2	D	617/637 (97%)	594 (96%)	21 (3%)	2 (0%)	36	42
All	All	2684/2728 (98%)	2584 (96%)	97 (4%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	435	THR
2	D	171	ASP
2	B	603	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	582/590 (99%)	567 (97%)	15 (3%)	40	55
1	C	582/590 (99%)	565 (97%)	17 (3%)	37	51
2	B	483/509 (95%)	466 (96%)	17 (4%)	32	43
2	D	483/509 (95%)	461 (95%)	22 (5%)	24	32
All	All	2130/2198 (97%)	2059 (97%)	71 (3%)	33	45

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	THR
1	A	4	LEU
1	A	24	ARG
1	A	26	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	31	LYS
1	A	36	GLU
1	A	67	ILE
1	A	69	PRO
1	A	202	LYS
1	A	567	SER
1	A	597	ARG
1	A	668	LEU
1	A	670	LYS
1	A	691	GLN
2	B	20	THR
2	B	75	MET
2	B	79	LYS
2	B	83	LYS
2	B	163	LYS
2	B	216	VAL
2	B	279	THR
2	B	334	GLU
2	B	410	ARG
2	B	431	LYS
2	B	435	THR
2	B	436	GLU
2	B	440	LYS
2	B	505	THR
2	B	512	LYS
2	B	629	SER
2	B	638	LYS
1	C	3	THR
1	C	4	LEU
1	C	24	ARG
1	C	31	LYS
1	C	51	ASN
1	C	67	ILE
1	C	69	PRO
1	C	202	LYS
1	C	327	THR
1	C	365	THR
1	C	384	ARG
1	C	498	LYS
1	C	533	LYS
1	C	577	THR
1	C	596	ARG

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Mol	Chain	Res	Type
1	C	668	LEU
1	C	691	GLN
2	D	20	THR
2	D	22	SER
2	D	77	ARG
2	D	79	LYS
2	D	83	LYS
2	D	156	ASP
2	D	158	LEU
2	D	187	ASP
2	D	216	VAL
2	D	322	GLN
2	D	334	GLU
2	D	336	PRO
2	D	358	ILE
2	D	410	ARG
2	D	431	LYS
2	D	436	GLU
2	D	477	LYS
2	D	501	MET
2	D	532	SER
2	D	586	LYS
2	D	616	ARG
2	D	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	215	GLN
1	A	359	HIS
1	A	385	ASN
1	A	462	GLN
1	A	492	GLN
1	A	643	GLN
1	A	691	GLN
2	B	239	ASN
2	B	323	ASN
2	B	563	GLN
2	B	577	GLN
1	C	359	HIS
1	C	385	ASN

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Mol	Chain	Res	Type
1	C	462	GLN
1	C	492	GLN
1	C	643	GLN
1	C	691	GLN
2	D	149	HIS
2	D	322	GLN
2	D	323	ASN
2	D	421	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 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	B12	A	1800	1	94,101,101	1.30	11 (11%)	149,166,166	2.06	42 (28%)
3	3CP	C	2801	-	54,56,56	1.55	9 (16%)	77,82,82	1.61	12 (15%)
5	GOL	C	3002	-	5,5,5	0.49	0	5,5,5	0.70	0
4	B12	C	2800	1	94,101,101	1.13	8 (8%)	149,166,166	1.88	36 (24%)
3	3CP	A	1801	-	54,56,56	1.29	6 (11%)	77,82,82	1.69	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	3001	-	5,5,5	0.65	0	5,5,5	1.13	1 (20%)

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	B12	A	1800	1	-	9/56/223/223	0/3/11/11
3	3CP	C	2801	-	-	8/54/70/70	0/3/3/3
5	GOL	C	3002	-	-	0/4/4/4	-
4	B12	C	2800	1	-	10/56/223/223	0/3/11/11
3	3CP	A	1801	-	-	7/54/70/70	0/3/3/3
5	GOL	A	3001	-	-	0/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2801	3CP	P1-O6	6.50	1.66	1.59
3	A	1801	3CP	P2-O6	4.84	1.64	1.59
4	A	1800	B12	C54-C17	4.04	1.61	1.54
3	C	2801	3CP	CP2-NP1	3.81	1.54	1.46
4	A	1800	B12	C14-N23	3.69	1.40	1.35
3	A	1801	3CP	CP5-NP2	3.58	1.54	1.46
4	A	1800	B12	C35-C5	3.49	1.57	1.50
4	A	1800	B12	C19-N24	-3.35	1.45	1.49
4	C	2800	B12	C48-C13	3.20	1.61	1.54
4	C	2800	B12	C54-C17	2.94	1.59	1.54
4	C	2800	B12	C14-N23	2.92	1.39	1.35
3	A	1801	3CP	C2-N1	2.83	1.39	1.33
3	A	1801	3CP	CP2-NP1	2.82	1.52	1.46
4	A	1800	B12	C41-C8	2.69	1.60	1.54
4	A	1800	B12	C2B-N1B	-2.68	1.33	1.37
4	A	1800	B12	O8R-C5R	2.68	1.53	1.42
4	C	2800	B12	C19-N24	-2.58	1.46	1.49
4	C	2800	B12	C55-C17	-2.53	1.49	1.54
3	A	1801	3CP	P2-O7	-2.51	1.49	1.59
3	C	2801	3CP	P2-O7	-2.49	1.49	1.59
3	C	2801	3CP	CP9-CPA	-2.48	1.48	1.53
3	C	2801	3CP	P1-O11	-2.42	1.42	1.50
3	C	2801	3CP	CP5-NP2	2.40	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2800	B12	C41-C8	2.35	1.59	1.54
4	A	1800	B12	C55-C17	-2.35	1.49	1.54
4	A	1800	B12	C55-C56	2.30	1.58	1.53
3	C	2801	3CP	P2-O6	2.27	1.62	1.59
4	C	2800	B12	C30-C3	2.25	1.59	1.54
4	A	1800	B12	P-O2	2.21	1.66	1.59
3	C	2801	3CP	C2-N1	2.19	1.37	1.33
3	A	1801	3CP	P2-O22	-2.19	1.45	1.55
3	C	2801	3CP	C2-N3	-2.11	1.30	1.33
4	C	2800	B12	C2B-N1B	-2.03	1.34	1.37
4	A	1800	B12	C13-C14	-2.01	1.48	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	3CP	CP8-CPA-CPB	6.81	119.46	108.22
3	C	2801	3CP	CP9-CPA-CPB	6.26	118.55	108.22
4	A	1800	B12	C9B-C8B-N1B	6.23	108.06	105.30
4	A	1800	B12	C20-C1-C19	6.02	115.14	109.35
4	A	1800	B12	C19-N24-C16	5.95	113.80	107.29
4	C	2800	B12	C19-N24-C16	5.81	113.64	107.29
3	A	1801	3CP	CP1-CP2-NP1	-5.72	100.48	112.41
4	C	2800	B12	C55-C17-C16	5.28	126.91	116.59
4	A	1800	B12	C55-C17-C18	5.18	121.00	111.12
4	A	1800	B12	C54-C17-C16	-4.80	87.53	112.41
4	A	1800	B12	C15-C16-N24	4.77	129.21	122.42
4	A	1800	B12	C10-C9-N22	-4.59	120.51	125.74
4	C	2800	B12	C1P-N59-C57	-4.44	113.16	122.69
4	C	2800	B12	C41-C8-C9	-4.42	103.47	111.19
3	A	1801	3CP	CP5-NP2-CP6	-4.40	114.65	122.55
4	A	1800	B12	C16-C15-C14	-4.39	114.56	121.26
4	C	2800	B12	C16-C15-C14	-4.25	114.78	121.26
3	C	2801	3CP	CP8-CPA-CPB	4.24	115.23	108.22
4	C	2800	B12	C36-C7-C8	4.23	119.86	112.05
4	C	2800	B12	C9B-C8B-N1B	4.12	107.13	105.30
4	C	2800	B12	C54-C17-C16	-4.03	91.54	112.41
3	C	2801	3CP	CS2-CS3-CS4	-3.91	104.30	114.51
4	C	2800	B12	C20-C1-C19	3.86	113.07	109.35
3	A	1801	3CP	CP9-CPA-CPB	3.84	114.57	108.22
4	C	2800	B12	C9-N22-C6	3.84	109.89	105.28
4	A	1800	B12	C55-C56-C57	-3.79	102.79	111.25
4	C	2800	B12	O44-C43-N45	-3.61	112.88	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2801	3CP	CP5-NP2-CP6	-3.60	116.07	122.55
4	A	1800	B12	C13-C14-N23	3.50	113.83	109.09
3	A	1801	3CP	O7-CPB-CPA	-3.50	104.93	110.55
4	A	1800	B12	C1-C19-N24	-3.45	102.41	106.25
4	A	1800	B12	O28-C27-N29	-3.45	113.33	122.53
4	C	2800	B12	C8B-C9B-N3B	-3.39	106.33	110.00
3	C	2801	3CP	CP1-CP2-NP1	-3.37	105.39	112.41
4	A	1800	B12	C8B-C9B-N3B	-3.34	106.39	110.00
3	A	1801	3CP	CP2-NP1-CP3	-3.32	116.63	122.82
4	C	2800	B12	C56-C55-C17	-3.30	109.21	115.58
4	C	2800	B12	C4B-C9B-N3B	3.29	136.04	130.51
3	C	2801	3CP	O7-CPB-CPA	-3.28	105.28	110.55
4	A	1800	B12	C36-C7-C8	3.27	118.08	112.05
4	C	2800	B12	C18-C17-C16	3.27	104.63	100.69
4	A	1800	B12	C41-C8-C9	-3.26	105.50	111.19
4	A	1800	B12	C13-C14-C15	-3.24	119.39	124.32
4	C	2800	B12	C15-C16-N24	3.22	127.01	122.42
4	A	1800	B12	C10-C11-N23	3.16	129.76	124.42
4	A	1800	B12	O58-C57-N59	3.14	129.18	123.03
4	A	1800	B12	C18-C17-C16	3.12	104.45	100.69
4	C	2800	B12	C42-C43-N45	3.12	126.48	116.49
4	C	2800	B12	O34-C32-C31	-3.10	111.67	121.04
3	A	1801	3CP	CS2-CS3-CS4	-3.10	106.42	114.51
4	C	2800	B12	C9B-N3B-C2B	3.06	108.15	104.40
4	A	1800	B12	C12-C11-C10	-3.00	119.53	123.40
4	A	1800	B12	C41-C8-C7	-2.97	106.02	114.19
4	C	2800	B12	C54-C17-C55	-2.97	104.33	109.27
4	A	1800	B12	C7-C6-C5	-2.96	123.44	128.07
4	A	1800	B12	C48-C13-C12	-2.96	108.05	116.52
4	A	1800	B12	O3-C2P-C1P	-2.92	101.16	106.94
4	A	1800	B12	C30-C3-C4	2.91	116.48	109.66
4	C	2800	B12	C18-C19-N24	2.91	106.70	102.33
4	A	1800	B12	C35-C5-C6	-2.81	117.88	122.41
4	C	2800	B12	C55-C17-C18	2.78	116.42	111.12
4	C	2800	B12	C4B-C9B-C8B	-2.77	117.62	120.16
4	A	1800	B12	C12-C13-C14	-2.76	97.72	102.26
3	A	1801	3CP	CP9-CPA-CP7	-2.76	104.06	108.77
4	A	1800	B12	C7-C6-N22	2.73	112.92	107.94
4	C	2800	B12	O58-C57-N59	2.73	128.39	123.03
4	A	1800	B12	C9-C10-C11	-2.73	122.07	125.97
4	C	2800	B12	C49-C50-N52	2.72	125.21	116.49
4	C	2800	B12	C54-C17-C18	-2.66	109.17	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2800	B12	C55-C56-C57	-2.65	105.34	111.25
4	C	2800	B12	C36-C7-C37	-2.64	106.25	110.74
4	A	1800	B12	C3-C4-N21	2.60	115.21	111.98
3	A	1801	3CP	OS5-CS4-OS4	-2.57	116.71	123.33
3	C	2801	3CP	O32-P3-O31	2.54	120.75	110.83
4	A	1800	B12	C7-C8-C9	2.54	104.11	100.89
4	A	1800	B12	C2-C1-C19	-2.54	114.67	118.61
3	C	2801	3CP	CP8-CPA-CP9	-2.52	104.17	109.20
4	C	2800	B12	C2-C1-C19	-2.51	114.71	118.61
4	C	2800	B12	C53-C15-C16	2.47	124.56	120.36
4	A	1800	B12	C37-C7-C8	-2.45	101.91	108.37
4	C	2800	B12	C49-C48-C13	-2.41	107.81	114.65
3	C	2801	3CP	OP2-CP6-NP2	2.41	128.09	122.98
4	A	1800	B12	C18-C19-N24	2.37	105.90	102.33
4	C	2800	B12	O7R-C2R-C1R	2.34	118.18	110.10
3	A	1801	3CP	CP8-CPA-CP9	-2.34	104.54	109.20
4	A	1800	B12	O58-C57-C56	-2.31	117.83	122.02
4	A	1800	B12	O44-C43-N45	-2.25	116.53	122.53
4	C	2800	B12	C1-C19-C18	-2.21	118.33	121.90
4	A	1800	B12	C17-C16-N24	-2.19	107.83	111.17
3	C	2801	3CP	OP1-CP3-CP4	-2.17	118.08	122.02
4	C	2800	B12	C4R-O6R-C1R	-2.15	104.73	109.47
4	A	1800	B12	C53-C15-C16	2.14	124.00	120.36
4	C	2800	B12	C31-C30-C3	-2.12	108.64	114.65
4	A	1800	B12	C17-C16-C15	-2.12	122.91	126.26
3	C	2801	3CP	C5-N7-C8	-2.10	100.16	103.45
5	A	3001	GOL	C3-C2-C1	-2.08	104.18	111.80
4	A	1800	B12	C26-C27-N29	2.08	122.92	116.49
4	A	1800	B12	C25-C2-C1	2.07	116.84	113.75
3	C	2801	3CP	CP9-CPA-CP7	-2.06	105.26	108.77
4	A	1800	B12	C60-C18-C19	-2.04	109.29	114.59
4	C	2800	B12	C31-C32-N33	2.02	122.95	116.49

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	3CP	P1-O6-P2-O7
3	C	2801	3CP	P1-O6-P2-O7
4	A	1800	B12	C42-C41-C8-C9
4	A	1800	B12	C2R-C1R-N1B-C2B
4	C	2800	B12	C2R-C1R-N1B-C2B

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Mol	Chain	Res	Type	Atoms
4	C	2800	B12	C42-C41-C8-C9
3	A	1801	3CP	S-CS1-CS2-CS3
3	C	2801	3CP	S-CS1-CS2-CS3
4	A	1800	B12	C16-C17-C55-C56
4	A	1800	B12	C2R-C1R-N1B-C8B
4	C	2800	B12	C2R-C1R-N1B-C8B
4	A	1800	B12	C30-C31-C32-O34
4	A	1800	B12	C30-C31-C32-N33
3	A	1801	3CP	CS1-CS2-CS3-CS4
4	A	1800	B12	O6R-C1R-N1B-C8B
4	C	2800	B12	O6R-C1R-N1B-C8B
3	A	1801	3CP	P2-O6-P1-O12
3	C	2801	3CP	P2-O6-P1-O12
3	C	2801	3CP	CP2-CP1-S-CS1
4	C	2800	B12	C30-C31-C32-N33
3	A	1801	3CP	CS2-CS3-CS4-OS4
3	A	1801	3CP	CS2-CS3-CS4-OS5
3	C	2801	3CP	CS2-CS3-CS4-OS4
4	C	2800	B12	C30-C31-C32-O34
3	C	2801	3CP	CS2-CS3-CS4-OS5
4	C	2800	B12	C55-C56-C57-O58
4	C	2800	B12	C55-C56-C57-N59
3	C	2801	3CP	P2-O6-P1-O11
4	A	1800	B12	C2P-O3-P-O4
4	C	2800	B12	C2P-O3-P-O4
4	C	2800	B12	C2P-O3-P-O5
3	A	1801	3CP	CP2-CP1-S-CS1
3	C	2801	3CP	C3'-O3'-P3-O32
4	A	1800	B12	C13-C48-C49-C50

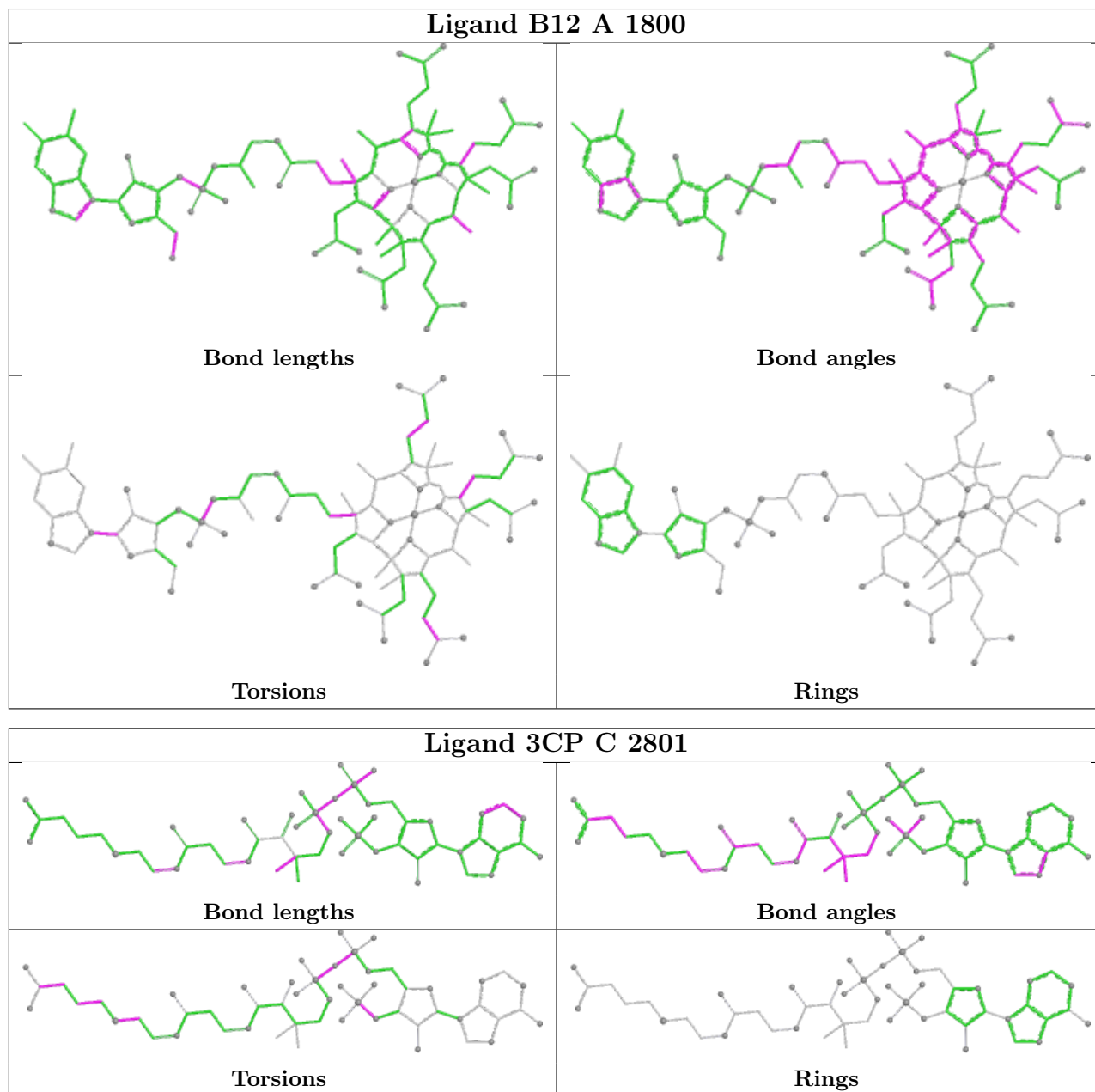
There are no ring outliers.

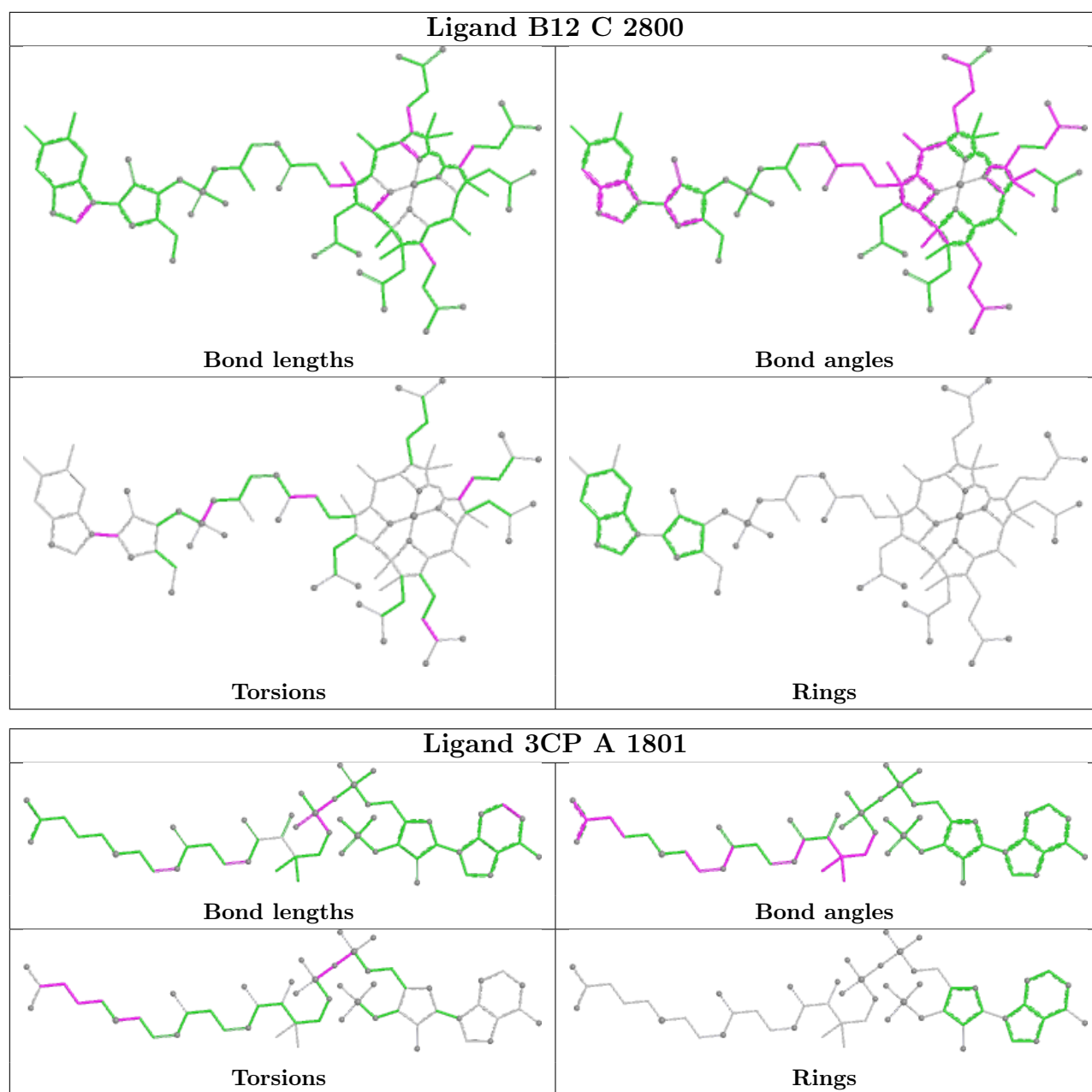
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1800	B12	12	0
3	C	2801	3CP	1	0
4	C	2800	B12	8	0
3	A	1801	3CP	1	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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	727/727 (100%)	-0.21	10 (1%) 73 71	16, 30, 53, 108	0
1	C	727/727 (100%)	-0.16	16 (2%) 62 59	14, 29, 53, 109	0
2	B	619/637 (97%)	0.08	16 (2%) 57 54	19, 37, 61, 93	0
2	D	619/637 (97%)	0.57	52 (8%) 17 14	19, 41, 64, 93	0
All	All	2692/2728 (98%)	0.05	94 (3%) 47 44	14, 33, 59, 109	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	107	TRP	6.0
1	C	23	ARG	5.4
2	D	305	ALA	5.2
1	C	728	ALA	5.1
2	B	107	TRP	4.8
2	D	106	ALA	4.5
2	D	270	GLY	4.5
1	C	2	SER	4.3
1	A	3	THR	4.1
1	C	3	THR	4.0
2	D	20	THR	4.0
1	A	728	ALA	3.8
2	B	106	ALA	3.8
1	A	2	SER	3.8
2	D	426	LEU	3.6
1	C	574	VAL	3.4
2	D	190	ALA	3.3
2	B	189	PRO	3.3
2	D	193	LEU	3.1
1	C	4	LEU	3.1
1	A	574	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	183	TYR	3.0
2	B	638	LYS	3.0
1	A	670	LYS	3.0
2	D	224	LEU	2.9
2	D	273	ALA	2.9
1	C	20	ASP	2.9
2	D	176	ALA	2.8
2	D	218	GLY	2.8
1	A	4	LEU	2.8
2	B	20	THR	2.7
1	C	15	ALA	2.7
2	B	188	LYS	2.7
2	D	25	GLY	2.7
2	D	116	PRO	2.7
2	D	105	ASP	2.6
2	D	189	PRO	2.6
2	B	190	ALA	2.6
2	D	81	ALA	2.6
1	C	727	ASP	2.6
2	D	219	ASP	2.6
2	D	274	THR	2.5
2	D	89	GLY	2.5
2	D	263	VAL	2.5
2	D	170	TYR	2.5
2	D	146	ALA	2.5
2	D	427	GLY	2.5
2	D	311	PHE	2.5
2	D	182	VAL	2.5
2	D	188	LYS	2.5
1	A	577	THR	2.4
1	C	576	ASN	2.4
2	B	603	GLY	2.4
2	D	312	GLY	2.4
2	D	217	LEU	2.4
2	D	230	ASP	2.4
2	D	222	ARG	2.4
2	D	272	THR	2.3
2	D	186	SER	2.3
2	D	214	LEU	2.3
2	D	266	LEU	2.3
2	D	178	ALA	2.3
1	C	17	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	426	LEU	2.3
2	B	105	ASP	2.3
2	B	48	PRO	2.3
2	B	155	SER	2.3
2	D	260	ALA	2.2
2	D	228	SER	2.2
2	D	227	PHE	2.2
2	B	216	VAL	2.2
2	D	164	VAL	2.2
1	A	676	GLY	2.2
1	C	36	GLU	2.2
2	D	191	LYS	2.2
2	D	276	ALA	2.2
1	C	16	PRO	2.2
2	D	173	GLY	2.2
1	A	429	LYS	2.1
2	D	91	ALA	2.1
2	D	174	ALA	2.1
2	D	638	LYS	2.1
2	D	50	GLU	2.1
1	A	576	ASN	2.1
2	D	313	VAL	2.1
1	C	577	THR	2.1
2	D	435	THR	2.1
2	D	150	LEU	2.0
2	B	185	ARG	2.0
2	D	267	VAL	2.0
1	C	35	GLY	2.0
2	B	425	LYS	2.0
2	B	186	SER	2.0
1	C	22	ALA	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](#)

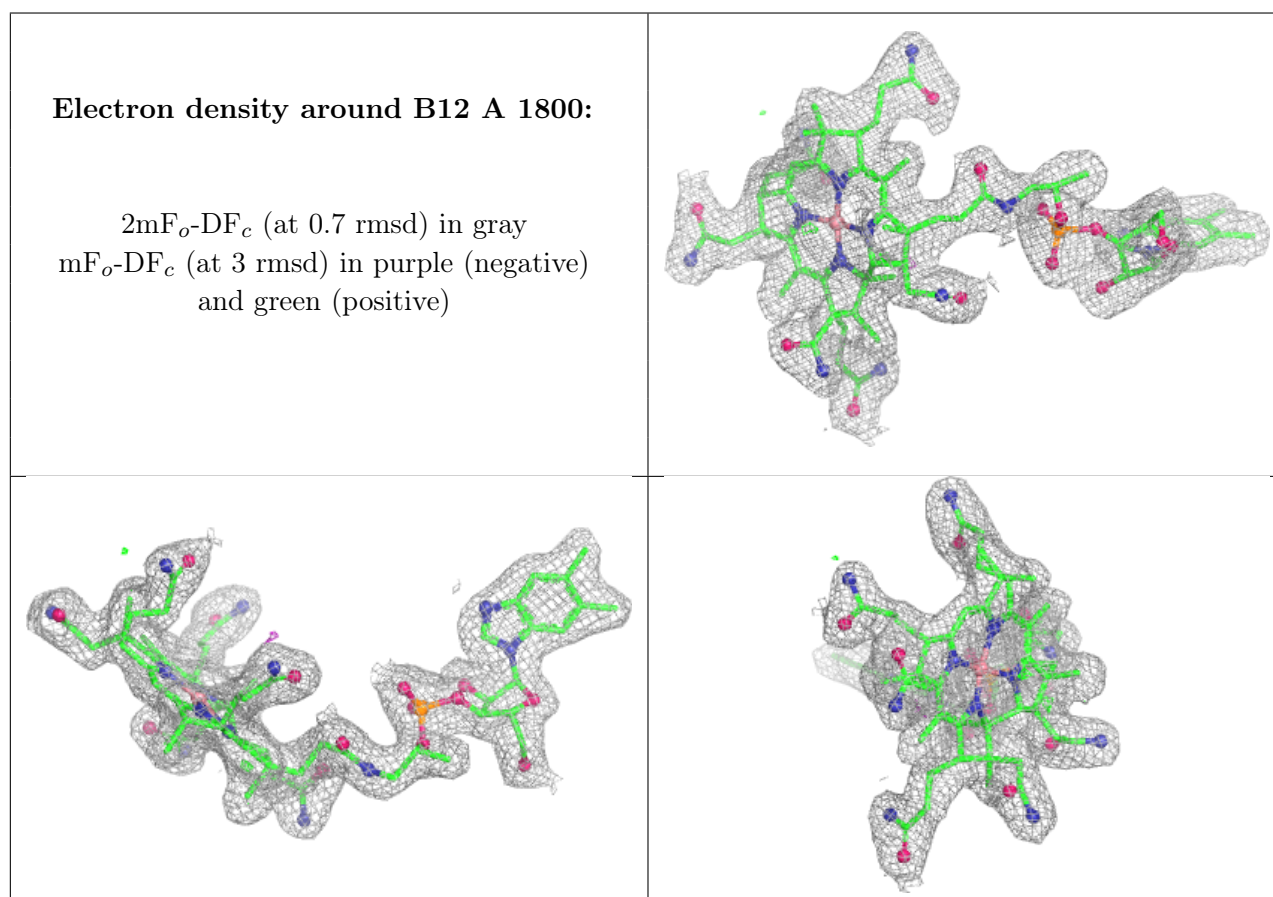
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

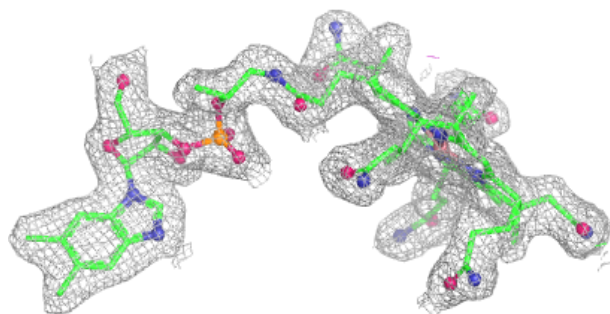
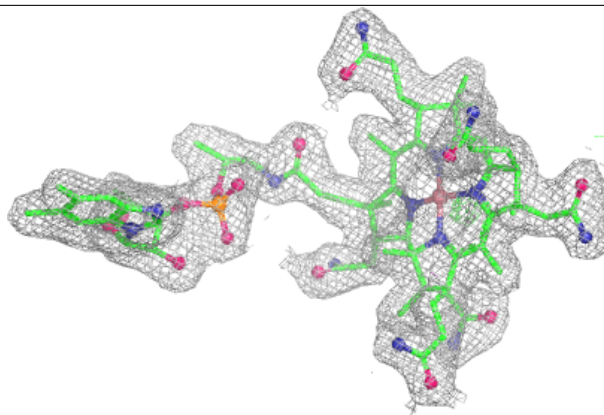
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	3001	6/6	0.92	0.10	29,34,37,40	0
5	GOL	C	3002	6/6	0.94	0.08	31,31,34,34	0
4	B12	A	1800	91/91	0.98	0.06	13,21,27,31	0
4	B12	C	2800	91/91	0.98	0.05	11,19,25,28	0
3	3CP	A	1801	54/54	0.98	0.06	17,24,31,35	0
3	3CP	C	2801	54/54	0.98	0.06	15,23,30,36	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.

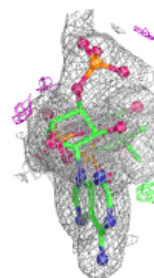
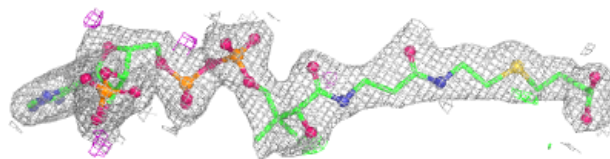
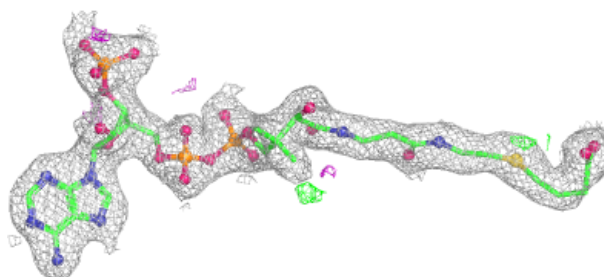


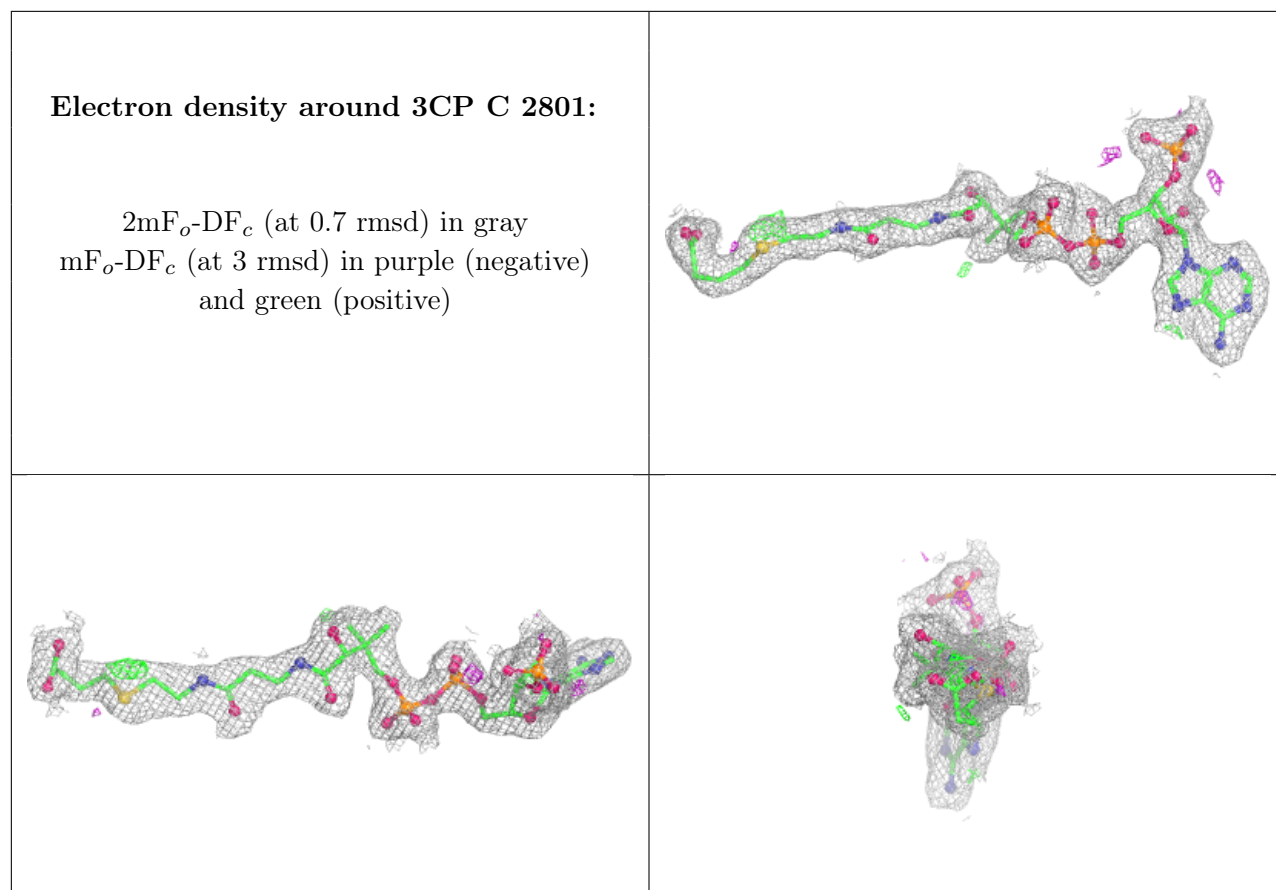
**Electron density around B12 C 2800:**

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

**Electron density around 3CP A 1801:**

$2mF_o-DF_c$  (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.