



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:14 AM UTC

PDB ID : 2REQ / pdb_00002req
Title : METHYLMALONYL-COA MUTASE, NON-PRODUCTIVE COA COMPLEX, IN OPEN CONFORMATION REPRESENTING SUBSTRATE-FREE STATE
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1997-09-22
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

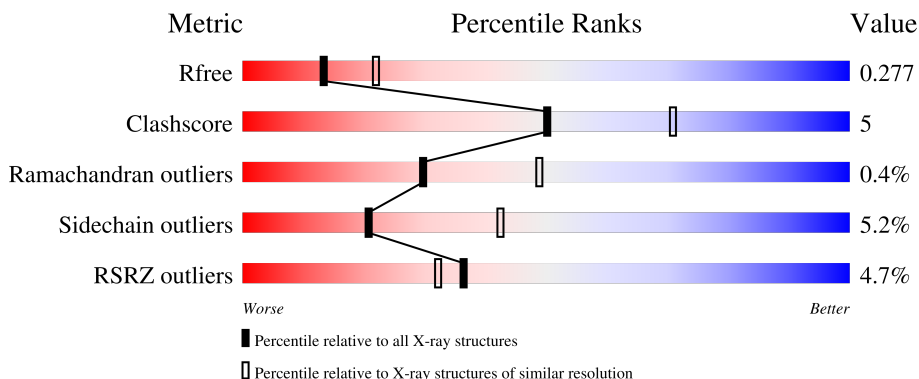
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

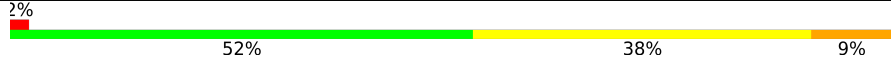

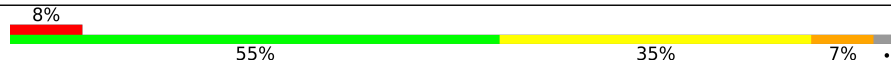

The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	727	 2% 52% 38% 9%
1	C	727	 3% 52% 39% 8%
2	B	637	 8% 55% 35% 7%
2	D	637	 6% 54% 35% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21240 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5564	3518	965	1057	24	0	0	0
1	C	725	5564	3518	965	1057	24	0	0	0

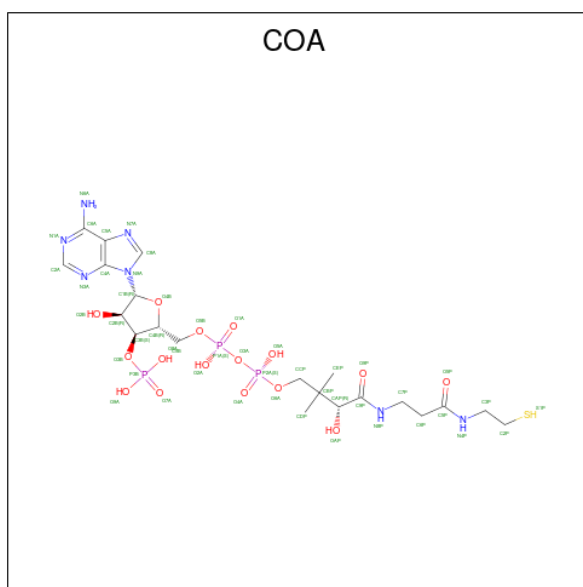
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	4616	2912	795	896	13	0	0	0
2	D	619	4616	2912	795	896	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

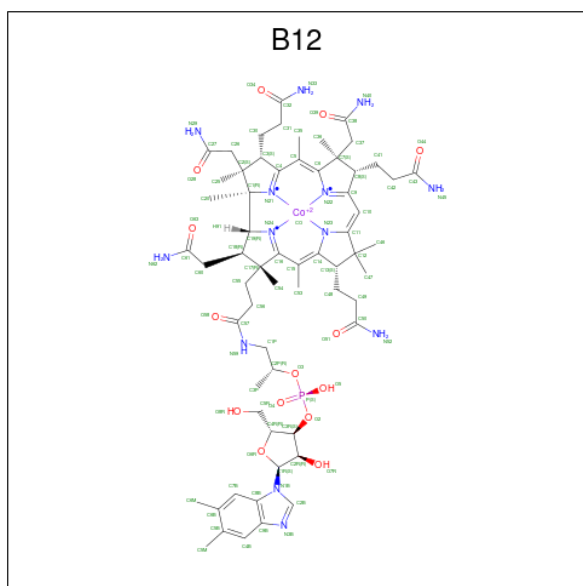
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0
3	C	1	31	10	5	13	3	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

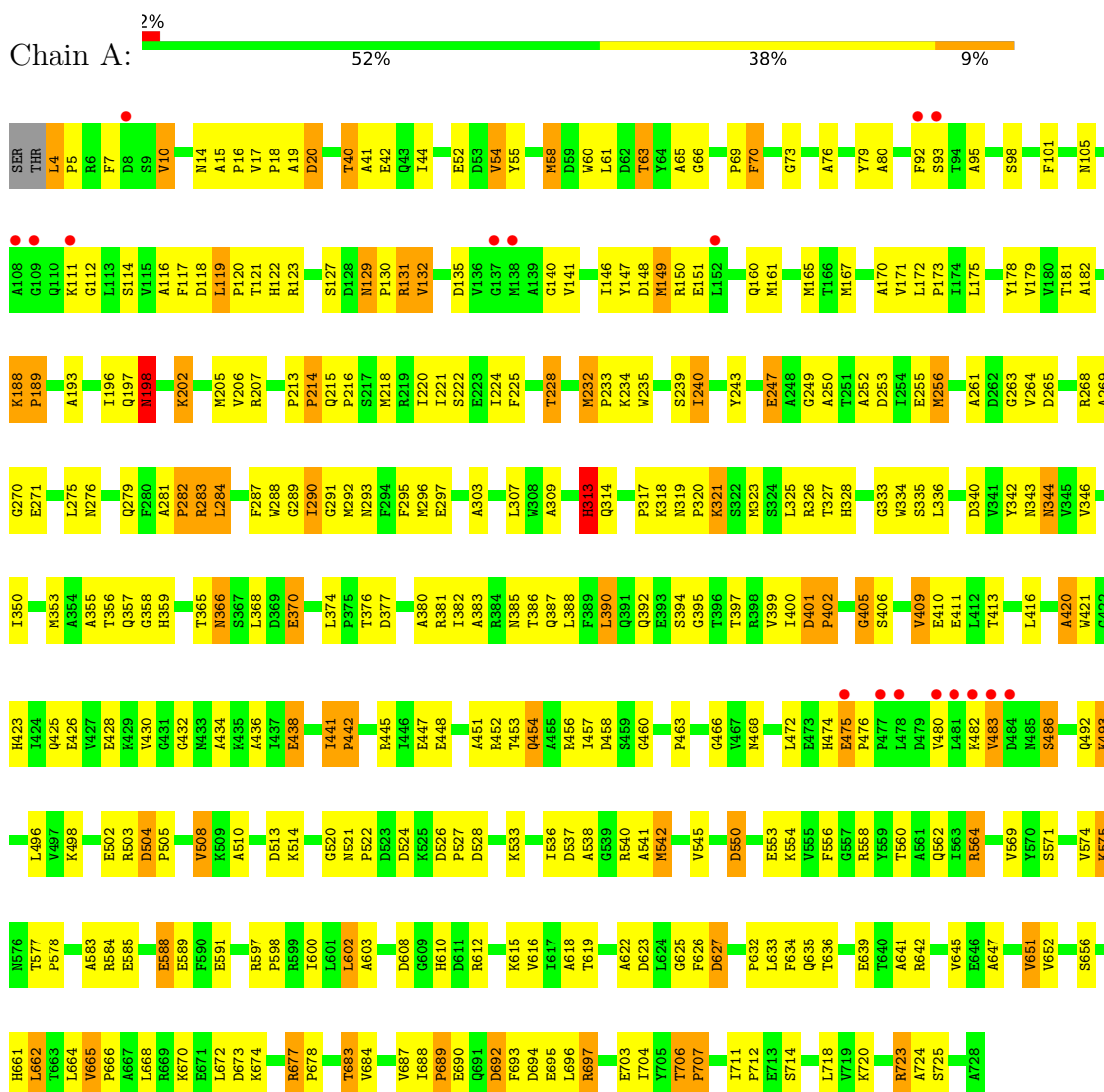
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0
5	B	112	Total 112	O 112	0	0
5	C	201	Total 201	O 201	0	0
5	D	117	Total 117	O 117	0	0

3 Residue-property plots i

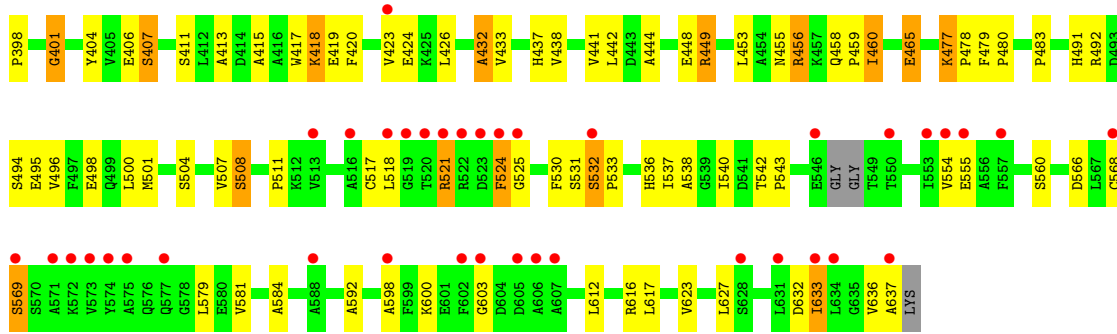
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

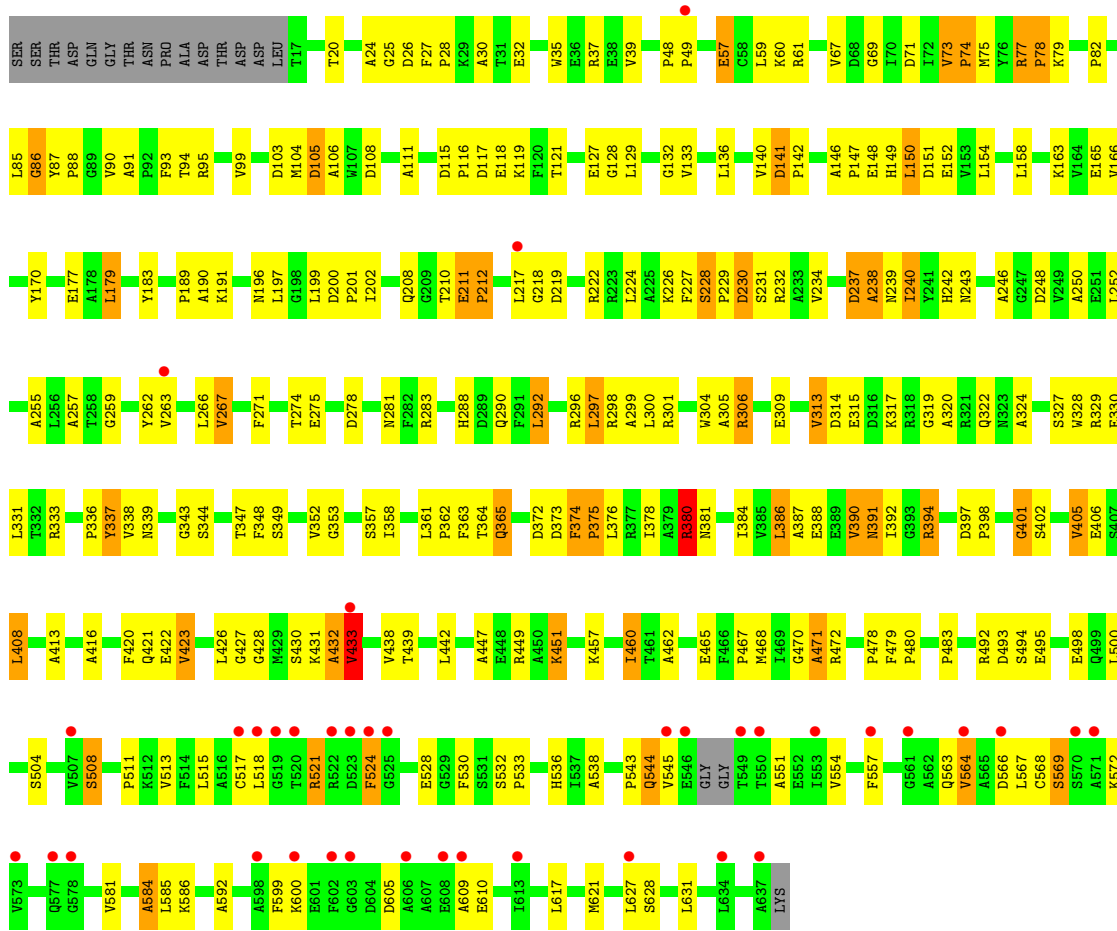


• Molecule 1: METHYLMALONYL-COA MUTASE





• Molecule 2: METHYLMALONYL-COA MUTASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.95Å 162.06Å 104.20Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 99.6 (20.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.50Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.259 , 0.325 0.224 , 0.277	Depositor DCC
R_{free} test set	4538 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtrriage
Anisotropy	0.185	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.009 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21240	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.86	1/5680 (0.0%)	2.54	483/7715 (6.3%)
1	C	0.90	1/5680 (0.0%)	2.59	515/7715 (6.7%)
2	B	0.78	0/4706	2.42	348/6414 (5.4%)
2	D	0.75	0/4706	2.43	353/6414 (5.5%)
All	All	0.83	2/20772 (0.0%)	2.50	1699/28258 (6.0%)

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	19
1	C	0	23
2	B	0	18
2	D	0	10
All	All	0	70

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	422	GLY	N-CA	-5.10	1.39	1.45
1	A	42	GLU	N-CA	-5.07	1.39	1.46

All (1699) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	ARG	CD-NE-CZ	20.98	153.77	124.40
1	A	540	ARG	CD-NE-CZ	15.21	145.69	124.40
2	B	335	ASP	CA-CB-CG	14.76	127.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	ILE	CB-CA-C	14.67	127.14	110.41
2	D	420	PHE	CA-CB-CG	13.86	127.66	113.80
1	C	189	PRO	CA-C-N	13.33	139.84	120.38
1	C	189	PRO	C-N-CA	13.33	139.84	120.38
1	C	699	ASP	CA-CB-CG	13.06	125.66	112.60
2	D	460	ILE	CB-CA-C	12.95	125.17	110.41
1	A	633	LEU	O-C-N	-12.83	107.55	122.68
2	B	524	PHE	CA-CB-CG	12.71	126.51	113.80
1	C	70	PHE	CA-CB-CG	12.61	126.41	113.80
2	D	524	PHE	CA-CB-CG	12.37	126.17	113.80
1	C	421	TRP	CA-C-N	12.28	133.32	119.94
1	C	421	TRP	C-N-CA	12.28	133.32	119.94
1	A	41	ALA	CA-C-N	12.26	141.19	120.72
1	A	41	ALA	C-N-CA	12.26	141.19	120.72
1	A	70	PHE	CA-CB-CG	12.17	125.97	113.80
1	C	578	PRO	CA-C-N	12.10	136.49	120.28
1	C	578	PRO	C-N-CA	12.10	136.49	120.28
2	B	390	VAL	CA-C-O	11.81	130.53	119.20
2	D	86	GLY	CA-C-O	11.77	130.35	122.23
2	B	390	VAL	O-C-N	-11.47	110.98	122.23
1	C	584	ARG	CD-NE-CZ	11.46	140.44	124.40
1	A	333	GLY	CA-C-N	11.18	135.26	120.28
1	A	333	GLY	C-N-CA	11.18	135.26	120.28
1	C	633	LEU	O-C-N	-11.15	109.53	122.68
2	D	390	VAL	CA-C-O	11.06	129.82	119.20
2	D	200	ASP	CA-CB-CG	11.00	123.60	112.60
1	C	92	PHE	CA-C-N	10.93	136.02	120.28
1	C	92	PHE	C-N-CA	10.93	136.02	120.28
1	A	263	GLY	CA-C-N	10.90	134.30	120.56
1	A	263	GLY	C-N-CA	10.90	134.30	120.56
2	D	390	VAL	O-C-N	-10.73	111.71	122.23
1	C	170	ALA	CA-C-N	10.72	135.65	120.42
1	C	170	ALA	C-N-CA	10.72	135.65	120.42
1	A	405	GLY	O-C-N	-10.61	111.61	122.65
1	A	111	LYS	CA-C-N	10.57	130.07	119.92
1	A	111	LYS	C-N-CA	10.57	130.07	119.92
1	C	540	ARG	NE-CZ-NH2	10.50	128.65	119.20
1	C	283	ARG	CD-NE-CZ	10.49	139.09	124.40
1	A	189	PRO	CA-C-N	10.42	135.60	120.38
1	A	189	PRO	C-N-CA	10.42	135.60	120.38
1	C	428	GLU	CA-C-N	10.38	133.93	120.44
1	C	428	GLU	C-N-CA	10.38	133.93	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLU	CA-CB-CG	10.30	134.70	114.10
2	D	32	GLU	CA-C-N	10.19	134.34	120.38
2	D	32	GLU	C-N-CA	10.19	134.34	120.38
1	C	118	ASP	CA-CB-CG	10.10	122.70	112.60
1	C	679	ASP	CA-C-O	-10.07	109.88	120.55
2	B	363	PHE	CA-C-N	9.94	136.51	120.60
2	B	363	PHE	C-N-CA	9.94	136.51	120.60
2	D	238	ALA	CA-C-N	9.93	133.59	120.28
2	D	238	ALA	C-N-CA	9.93	133.59	120.28
1	A	118	ASP	CA-CB-CG	9.91	122.51	112.60
2	D	600	LYS	CA-C-N	9.87	137.57	122.37
2	D	600	LYS	C-N-CA	9.87	137.57	122.37
1	C	320	PRO	CA-C-N	9.78	136.25	120.60
1	C	320	PRO	C-N-CA	9.78	136.25	120.60
2	D	343	GLY	CA-C-N	9.77	133.15	120.44
2	D	343	GLY	C-N-CA	9.77	133.15	120.44
1	C	345	VAL	CA-C-N	9.75	133.03	120.56
1	C	345	VAL	C-N-CA	9.75	133.03	120.56
2	D	304	TRP	CA-C-N	9.71	134.09	120.29
2	D	304	TRP	C-N-CA	9.71	134.09	120.29
1	A	528	ASP	CA-C-N	9.69	138.10	121.14
1	A	528	ASP	C-N-CA	9.69	138.10	121.14
2	D	337	TYR	O-C-N	-9.66	110.92	122.22
1	A	678	PRO	CA-C-N	9.57	133.11	120.28
1	A	678	PRO	C-N-CA	9.57	133.11	120.28
2	D	147	PRO	CA-C-N	9.57	133.11	120.28
2	D	147	PRO	C-N-CA	9.57	133.11	120.28
2	D	154	LEU	CA-C-N	9.54	133.43	120.54
2	D	154	LEU	C-N-CA	9.54	133.43	120.54
2	B	338	VAL	O-C-N	-9.54	110.65	122.57
1	A	458	ASP	CA-CB-CG	9.49	122.09	112.60
1	C	262	ASP	CA-C-N	9.44	130.66	119.99
1	C	262	ASP	C-N-CA	9.44	130.66	119.99
2	B	78	PRO	O-C-N	-9.44	111.39	122.24
2	B	86	GLY	O-C-N	-9.43	110.45	122.70
2	D	78	PRO	CA-C-N	9.43	135.68	120.60
2	D	78	PRO	C-N-CA	9.43	135.68	120.60
2	B	141	ASP	CA-CB-CG	9.42	122.02	112.60
1	C	493	LYS	CA-C-N	9.40	133.64	120.29
1	C	493	LYS	C-N-CA	9.40	133.64	120.29
1	C	384	ARG	NE-CZ-NH2	-9.38	110.76	119.20
1	C	420	ALA	CA-C-N	9.32	132.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	ALA	C-N-CA	9.32	132.77	120.28
1	A	411	GLU	O-C-N	-9.30	112.26	122.12
2	D	380	ARG	CD-NE-CZ	9.29	137.40	124.40
1	C	408	TYR	CA-C-N	9.20	133.07	120.46
1	C	408	TYR	C-N-CA	9.20	133.07	120.46
2	B	89	GLY	CA-C-N	9.19	136.67	122.25
2	B	89	GLY	C-N-CA	9.19	136.67	122.25
2	B	154	LEU	CA-C-N	9.17	132.93	120.54
2	B	154	LEU	C-N-CA	9.17	132.93	120.54
1	A	243	TYR	CA-C-N	9.10	132.82	120.54
1	A	243	TYR	C-N-CA	9.10	132.82	120.54
2	D	24	ALA	CA-C-N	9.06	131.55	120.13
2	D	24	ALA	C-N-CA	9.06	131.55	120.13
2	B	147	PRO	CA-C-N	9.05	133.31	120.28
2	B	147	PRO	C-N-CA	9.05	133.31	120.28
2	D	95	ARG	CG-CD-NE	9.04	131.90	112.00
1	C	182	ALA	CA-C-N	8.98	133.96	120.31
1	C	182	ALA	C-N-CA	8.98	133.96	120.31
2	D	117	ASP	CA-CB-CG	8.91	121.51	112.60
2	B	420	PHE	CA-CB-CG	8.88	122.68	113.80
1	C	56	LYS	CA-C-O	-8.88	110.63	121.02
1	C	215	GLN	O-C-N	-8.87	112.37	120.71
2	D	78	PRO	O-C-N	-8.83	112.08	122.24
1	A	319	ASN	CA-C-O	8.83	125.85	119.32
1	C	92	PHE	CA-C-O	8.82	130.73	121.38
1	A	706	THR	O-C-N	-8.78	114.82	121.14
1	A	270	GLY	CA-C-N	8.77	133.64	120.31
1	A	270	GLY	C-N-CA	8.77	133.64	120.31
2	B	397	ASP	CA-C-N	8.77	128.93	119.28
2	B	397	ASP	C-N-CA	8.77	128.93	119.28
2	B	200	ASP	CA-CB-CG	8.75	121.35	112.60
2	D	333	ARG	CD-NE-CZ	8.73	136.62	124.40
2	B	78	PRO	CA-C-N	8.72	134.55	120.60
2	B	78	PRO	C-N-CA	8.72	134.55	120.60
2	D	86	GLY	O-C-N	-8.67	112.58	122.64
2	D	296	ARG	CA-C-O	-8.64	111.26	120.42
2	D	85	LEU	CA-C-O	-8.63	111.27	120.42
1	A	179	VAL	CA-C-N	8.60	132.63	120.42
1	A	179	VAL	C-N-CA	8.60	132.63	120.42
1	C	79	TYR	CA-C-N	8.59	131.79	120.28
1	C	79	TYR	C-N-CA	8.59	131.79	120.28
2	B	104	MET	CA-C-N	8.58	137.85	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	MET	C-N-CA	8.58	137.85	122.31
1	A	545	VAL	CA-C-N	8.56	129.45	119.94
1	A	545	VAL	C-N-CA	8.56	129.45	119.94
1	C	287	PHE	CA-CB-CG	8.54	122.34	113.80
2	B	349	SER	O-C-N	-8.53	113.08	122.12
1	A	283	ARG	CD-NE-CZ	8.47	136.26	124.40
1	A	147	TYR	CA-C-N	8.45	131.95	120.54
1	A	147	TYR	C-N-CA	8.45	131.95	120.54
2	B	95	ARG	CG-CD-NE	8.43	130.55	112.00
1	A	101	PHE	CA-CB-CG	8.43	122.23	113.80
1	A	677	ARG	O-C-N	-8.43	114.55	121.12
2	B	330	GLU	CA-C-O	-8.36	109.49	119.27
1	C	319	ASN	OD1-CG-ND2	-8.25	114.35	122.60
1	C	490	ALA	CA-C-N	8.25	131.33	120.28
1	C	490	ALA	C-N-CA	8.25	131.33	120.28
1	A	633	LEU	CA-C-N	8.24	135.47	122.61
1	A	633	LEU	C-N-CA	8.24	135.47	122.61
1	C	508	VAL	CB-CA-C	-8.22	100.88	112.22
2	B	401	GLY	O-C-N	-8.21	112.02	122.70
1	A	536	ILE	CA-C-O	-8.21	112.88	121.41
1	C	545	VAL	CA-C-N	8.20	129.25	119.99
1	C	545	VAL	C-N-CA	8.20	129.25	119.99
2	B	117	ASP	CA-CB-CG	8.20	120.80	112.60
1	A	423	HIS	CA-C-N	8.18	131.67	120.46
1	A	423	HIS	C-N-CA	8.18	131.67	120.46
1	C	677	ARG	O-C-N	-8.18	114.61	121.23
2	B	69	GLY	N-CA-C	8.17	126.44	114.10
2	B	444	ALA	CA-C-N	8.17	131.23	120.28
2	B	444	ALA	C-N-CA	8.17	131.23	120.28
1	C	597	ARG	CD-NE-CZ	8.15	135.82	124.40
1	A	287	PHE	CA-CB-CG	8.14	121.94	113.80
1	C	633	LEU	CA-C-N	8.14	135.82	123.05
1	C	633	LEU	C-N-CA	8.14	135.82	123.05
1	C	689	PRO	CA-C-N	8.13	131.98	120.28
1	C	689	PRO	C-N-CA	8.13	131.98	120.28
1	A	314	GLN	CA-C-N	8.12	135.96	121.66
1	A	314	GLN	C-N-CA	8.12	135.96	121.66
2	B	264	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	A	677	ARG	CA-CB-CG	8.08	130.26	114.10
2	B	77	ARG	CA-C-N	8.08	128.53	119.32
2	B	77	ARG	C-N-CA	8.08	128.53	119.32
1	A	198	ASN	CA-CB-CG	8.07	120.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	VAL	CA-C-O	-8.06	110.70	120.78
2	D	301	ARG	CA-C-O	-8.04	112.03	120.55
1	A	356	THR	O-C-N	-8.02	112.40	122.27
2	B	424	GLU	CA-C-N	8.02	131.82	120.28
2	B	424	GLU	C-N-CA	8.02	131.82	120.28
1	A	7	PHE	CA-C-N	8.00	130.84	120.44
1	A	7	PHE	C-N-CA	8.00	130.84	120.44
2	B	32	GLU	CA-C-N	8.00	130.99	120.28
2	B	32	GLU	C-N-CA	8.00	130.99	120.28
1	C	147	TYR	CA-C-N	7.98	131.31	120.54
1	C	147	TYR	C-N-CA	7.98	131.31	120.54
1	A	504	ASP	CA-C-O	7.97	125.22	119.32
1	C	41	ALA	O-C-N	-7.96	112.91	122.22
1	A	626	PHE	CA-CB-CG	7.95	121.75	113.80
1	C	697	ARG	CA-C-N	7.94	130.77	120.44
1	C	697	ARG	C-N-CA	7.94	130.77	120.44
2	D	248	ASP	CA-CB-CG	7.94	120.54	112.60
1	C	504	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	215	GLN	CA-C-N	7.90	127.82	119.05
1	A	215	GLN	C-N-CA	7.90	127.82	119.05
1	A	633	LEU	CA-C-O	7.90	130.96	122.03
2	D	349	SER	O-C-N	-7.90	113.75	122.12
1	C	520	GLY	O-C-N	-7.87	112.79	122.71
1	C	175	LEU	CA-C-N	7.86	130.82	120.28
1	C	175	LEU	C-N-CA	7.86	130.82	120.28
1	C	63	THR	O-C-N	-7.85	113.74	122.84
2	D	93	PHE	O-C-N	-7.84	113.64	121.87
1	C	271	GLU	CA-C-N	7.83	131.56	120.28
1	C	271	GLU	C-N-CA	7.83	131.56	120.28
1	C	222	SER	CA-C-N	7.81	132.19	120.31
1	C	222	SER	C-N-CA	7.81	132.19	120.31
2	B	307	ILE	O-C-N	-7.77	114.33	121.87
1	A	571	SER	O-C-N	-7.76	114.02	122.09
2	D	566	ASP	CA-CB-CG	7.76	120.36	112.60
2	B	302	GLU	CB-CG-CD	7.73	125.74	112.60
2	B	146	ALA	CA-C-N	7.71	128.12	119.32
2	B	146	ALA	C-N-CA	7.71	128.12	119.32
2	B	382	THR	CA-C-N	7.71	128.50	119.94
2	B	382	THR	C-N-CA	7.71	128.50	119.94
1	C	217	SER	CA-C-N	7.70	130.59	120.28
1	C	217	SER	C-N-CA	7.70	130.59	120.28
1	A	127	SER	N-CA-C	7.69	121.92	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	610	HIS	CA-CB-CG	-7.69	106.11	113.80
1	A	538	ALA	CA-C-N	7.68	128.51	119.98
1	A	538	ALA	C-N-CA	7.68	128.51	119.98
1	C	79	TYR	O-C-N	-7.68	111.77	122.37
1	C	215	GLN	CA-C-O	7.67	125.78	118.34
1	A	521	ASN	OD1-CG-ND2	7.66	130.26	122.60
1	C	672	LEU	CA-C-N	7.66	133.70	120.68
1	C	672	LEU	C-N-CA	7.66	133.70	120.68
2	D	132	GLY	N-CA-C	7.64	125.52	115.36
1	C	623	ASP	CA-C-N	7.63	136.47	121.58
1	C	623	ASP	C-N-CA	7.63	136.47	121.58
1	C	42	GLU	CA-C-N	7.61	133.47	122.35
1	C	42	GLU	C-N-CA	7.61	133.47	122.35
2	D	151	ASP	CA-C-N	7.61	130.33	120.44
2	D	151	ASP	C-N-CA	7.61	130.33	120.44
2	D	397	ASP	CA-C-N	7.60	127.64	119.28
2	D	397	ASP	C-N-CA	7.60	127.64	119.28
1	A	674	LYS	CA-C-N	7.59	135.61	122.56
1	A	674	LYS	C-N-CA	7.59	135.61	122.56
2	B	238	ALA	CA-C-N	7.58	130.44	120.28
2	B	238	ALA	C-N-CA	7.58	130.44	120.28
1	C	562	GLN	OE1-CD-NE2	7.58	130.18	122.60
2	D	128	GLY	CA-C-O	-7.58	113.37	120.80
1	C	225	PHE	CA-CB-CG	7.58	121.38	113.80
1	A	591	GLU	CA-C-N	7.57	131.19	120.28
1	A	591	GLU	C-N-CA	7.57	131.19	120.28
2	B	432	ALA	CA-C-N	7.57	131.17	120.42
2	B	432	ALA	C-N-CA	7.57	131.17	120.42
1	C	252	ALA	N-CA-C	7.56	119.52	111.28
2	B	600	LYS	CA-C-N	7.56	134.01	122.37
2	B	600	LYS	C-N-CA	7.56	134.01	122.37
1	C	272	SER	O-C-N	-7.55	113.39	122.22
1	A	321	LYS	CA-C-N	7.55	131.01	120.29
1	A	321	LYS	C-N-CA	7.55	131.01	120.29
1	C	207	ARG	CA-C-O	7.55	128.10	119.27
1	C	229	SER	CA-C-N	7.54	130.88	120.63
1	C	229	SER	C-N-CA	7.54	130.88	120.63
2	B	337	TYR	CA-C-O	-7.53	111.59	120.10
1	C	249	GLY	CA-C-O	-7.52	110.54	119.04
2	D	79	LYS	CA-C-N	7.52	136.25	121.58
2	D	79	LYS	C-N-CA	7.52	136.25	121.58
2	D	449	ARG	CA-C-O	-7.51	112.94	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	MET	CA-C-N	7.51	130.95	120.29
1	A	296	MET	C-N-CA	7.51	130.95	120.29
2	B	122	ARG	CA-C-N	7.50	130.67	120.54
2	B	122	ARG	C-N-CA	7.50	130.67	120.54
1	C	397	THR	O-C-N	-7.49	111.77	122.41
2	D	292	LEU	CA-C-O	-7.49	112.61	120.55
1	C	626	PHE	CA-CB-CG	7.48	121.28	113.80
1	A	14	ASN	CA-C-O	7.46	128.98	119.95
2	D	69	GLY	CA-C-N	-7.46	113.53	122.93
2	D	69	GLY	C-N-CA	-7.46	113.53	122.93
1	C	335	SER	CA-C-O	-7.46	111.39	119.97
1	A	496	LEU	CA-C-N	7.45	129.81	120.72
1	A	496	LEU	C-N-CA	7.45	129.81	120.72
2	D	93	PHE	CA-C-N	7.45	130.59	120.38
2	D	93	PHE	C-N-CA	7.45	130.59	120.38
2	D	504	SER	N-CA-C	7.44	120.27	111.71
1	A	466	GLY	CA-C-N	7.44	130.26	122.97
1	A	466	GLY	C-N-CA	7.44	130.26	122.97
1	C	550	ASP	CA-C-N	7.43	130.56	120.54
1	C	550	ASP	C-N-CA	7.43	130.56	120.54
2	D	431	LYS	CA-C-N	7.42	130.55	120.38
2	D	431	LYS	C-N-CA	7.42	130.55	120.38
2	B	339	ASN	CA-C-N	7.42	129.90	120.56
2	B	339	ASN	C-N-CA	7.42	129.90	120.56
1	C	506	GLU	CA-C-N	7.41	130.21	120.28
1	C	506	GLU	C-N-CA	7.41	130.21	120.28
1	A	704	ILE	O-C-N	-7.41	115.35	123.20
1	C	54	VAL	CA-C-N	7.40	131.56	120.31
1	C	54	VAL	C-N-CA	7.40	131.56	120.31
1	C	379	SER	CA-C-N	7.39	130.92	120.28
1	C	379	SER	C-N-CA	7.39	130.92	120.28
1	A	636	THR	CA-C-N	7.38	126.91	119.24
1	A	636	THR	C-N-CA	7.38	126.91	119.24
1	C	647	ALA	CA-C-N	7.37	133.25	122.63
1	C	647	ALA	C-N-CA	7.37	133.25	122.63
1	A	334	TRP	CA-C-N	7.36	133.01	120.72
1	A	334	TRP	C-N-CA	7.36	133.01	120.72
1	C	689	PRO	N-CA-CB	7.35	109.85	103.31
1	A	60	TRP	O-C-N	-7.34	113.16	122.34
2	D	115	ASP	CA-C-N	7.33	126.59	118.97
2	D	115	ASP	C-N-CA	7.33	126.59	118.97
2	D	149	HIS	CA-C-N	7.33	130.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	149	HIS	C-N-CA	7.33	130.10	120.28
2	D	361	LEU	CA-C-O	7.33	127.70	120.23
1	A	55	TYR	N-CA-C	7.32	120.31	111.82
1	C	299	ALA	CA-C-N	7.31	130.41	120.54
1	C	299	ALA	C-N-CA	7.31	130.41	120.54
1	A	92	PHE	CA-C-N	7.31	132.29	120.60
1	A	92	PHE	C-N-CA	7.31	132.29	120.60
2	B	358	ILE	CB-CG1-CD1	7.30	129.13	113.80
1	A	289	GLY	CA-C-O	-7.30	114.76	121.18
2	B	283	ARG	NE-CZ-NH1	7.29	128.79	121.50
2	D	61	ARG	CD-NE-CZ	7.28	134.59	124.40
1	C	489	LEU	CA-C-N	7.27	130.32	120.44
1	C	489	LEU	C-N-CA	7.27	130.32	120.44
1	C	419	LYS	O-C-N	-7.26	114.59	122.07
2	D	401	GLY	O-C-N	-7.26	113.26	122.70
2	B	329	ARG	N-CA-C	7.25	120.05	111.71
2	D	25	GLY	O-C-N	-7.25	114.72	122.19
1	A	42	GLU	CA-C-N	7.25	135.38	121.54
1	A	42	GLU	C-N-CA	7.25	135.38	121.54
2	B	243	ASN	OD1-CG-ND2	-7.24	115.36	122.60
2	D	423	VAL	CA-C-N	7.23	131.30	120.31
2	D	423	VAL	C-N-CA	7.23	131.30	120.31
1	C	131	ARG	O-C-N	-7.22	113.97	122.20
2	B	424	GLU	O-C-N	-7.22	114.58	122.09
1	C	42	GLU	O-C-N	-7.22	112.50	122.46
1	C	370	GLU	CA-CB-CG	7.20	128.51	114.10
1	C	342	TYR	CA-C-O	-7.20	109.89	119.11
1	C	541	ALA	CA-C-N	7.20	132.86	122.35
1	C	541	ALA	C-N-CA	7.20	132.86	122.35
1	C	633	LEU	CA-C-O	7.19	130.15	122.03
1	C	476	PRO	N-CA-CB	7.18	106.95	103.22
2	D	406	GLU	CB-CG-CD	7.16	124.78	112.60
2	B	419	GLU	O-C-N	-7.16	114.53	122.12
2	D	48	PRO	CA-C-N	7.16	126.99	119.05
2	D	48	PRO	C-N-CA	7.16	126.99	119.05
1	C	526	ASP	CA-C-O	7.14	126.20	119.99
1	A	410	GLU	CB-CG-CD	7.14	124.74	112.60
2	D	90	VAL	CA-CB-CG2	7.14	122.54	110.40
1	A	441	ILE	CA-C-N	7.13	126.66	119.24
1	A	441	ILE	C-N-CA	7.13	126.66	119.24
1	A	627	ASP	O-C-N	-7.13	114.93	123.13
2	B	338	VAL	CA-C-N	7.13	133.61	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	VAL	C-N-CA	7.13	133.61	121.14
2	B	496	VAL	CA-C-N	7.12	131.14	120.31
2	B	496	VAL	C-N-CA	7.12	131.14	120.31
2	D	422	GLU	O-C-N	-7.12	114.68	122.09
2	D	462	ALA	CA-C-N	7.12	134.78	121.97
2	D	462	ALA	C-N-CA	7.12	134.78	121.97
2	D	73	VAL	CA-C-N	7.11	126.73	119.19
2	D	73	VAL	C-N-CA	7.11	126.73	119.19
2	D	305	ALA	CA-C-N	7.11	130.39	120.29
2	D	305	ALA	C-N-CA	7.11	130.39	120.29
2	B	318	ARG	CA-C-N	7.11	127.96	120.43
2	B	318	ARG	C-N-CA	7.11	127.96	120.43
1	C	216	PRO	CA-C-N	7.10	129.80	120.28
1	C	216	PRO	C-N-CA	7.10	129.80	120.28
1	A	537	ASP	O-C-N	-7.10	114.59	122.12
2	B	200	ASP	CA-C-N	7.09	126.62	119.24
2	B	200	ASP	C-N-CA	7.09	126.62	119.24
2	B	295	ALA	CA-C-N	7.09	129.78	120.28
2	B	295	ALA	C-N-CA	7.09	129.78	120.28
1	C	432	GLY	N-CA-C	-7.08	104.81	112.04
1	A	577	THR	CA-C-N	7.08	126.91	119.05
1	A	577	THR	C-N-CA	7.08	126.91	119.05
1	A	612	ARG	CA-C-N	7.07	127.79	119.94
1	A	612	ARG	C-N-CA	7.07	127.79	119.94
1	A	297	GLU	O-C-N	-7.07	114.09	122.15
2	D	384	ILE	CA-C-O	-7.07	113.68	121.17
1	A	678	PRO	N-CA-CB	7.06	110.03	103.46
1	C	513	ASP	O-C-N	-7.05	113.97	122.22
2	B	392	ILE	CA-C-O	-7.05	111.05	119.58
2	B	93	PHE	CA-C-N	7.04	130.05	120.54
2	B	93	PHE	C-N-CA	7.04	130.05	120.54
2	B	225	ALA	N-CA-C	7.03	119.79	111.71
1	C	589	GLU	CA-C-N	7.03	129.69	120.28
1	C	589	GLU	C-N-CA	7.03	129.69	120.28
1	C	677	ARG	CA-CB-CG	7.02	128.15	114.10
1	C	555	VAL	CA-C-O	-7.02	112.67	120.46
1	A	647	ALA	CA-C-N	7.02	132.32	122.36
1	A	647	ALA	C-N-CA	7.02	132.32	122.36
1	A	346	VAL	CB-CA-C	-7.02	102.54	112.22
2	D	521	ARG	CA-C-N	6.99	130.22	120.29
2	D	521	ARG	C-N-CA	6.99	130.22	120.29
1	C	452	ARG	NE-CZ-NH2	-6.99	112.91	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	586	LEU	O-C-N	-6.99	114.72	122.12
1	C	215	GLN	CA-C-N	6.98	126.80	119.05
1	C	215	GLN	C-N-CA	6.98	126.80	119.05
2	D	344	SER	N-CA-C	6.98	118.53	111.07
1	C	623	ASP	O-C-N	-6.97	113.08	122.43
1	C	269	ALA	CA-C-N	6.96	127.66	120.00
1	C	269	ALA	C-N-CA	6.96	127.66	120.00
1	C	277	VAL	O-C-N	-6.96	115.07	121.89
1	C	455	ALA	CA-C-O	-6.95	113.19	120.55
2	D	427	GLY	N-CA-C	6.95	123.12	114.37
2	B	307	ILE	CA-C-N	6.94	127.69	119.98
2	B	307	ILE	C-N-CA	6.94	127.69	119.98
2	B	349	SER	CA-C-N	6.94	129.46	120.44
2	B	349	SER	C-N-CA	6.94	129.46	120.44
1	A	690	GLU	CA-C-N	6.94	130.27	120.28
1	A	690	GLU	C-N-CA	6.94	130.27	120.28
2	D	536	HIS	O-C-N	-6.93	113.15	122.43
1	A	553	GLU	CA-C-N	6.92	129.89	120.54
1	A	553	GLU	C-N-CA	6.92	129.89	120.54
1	A	232	MET	CA-CB-CG	6.92	127.94	114.10
1	A	117	PHE	CA-C-O	6.92	129.20	121.11
2	B	68	ASP	CA-C-N	6.91	132.80	120.77
2	B	68	ASP	C-N-CA	6.91	132.80	120.77
2	D	333	ARG	N-CA-C	-6.91	103.49	112.68
1	A	520	GLY	O-C-N	-6.91	114.88	122.68
1	A	527	PRO	N-CA-CB	6.90	110.14	103.51
1	C	441	ILE	CA-C-N	6.90	126.14	118.97
1	C	441	ILE	C-N-CA	6.90	126.14	118.97
1	A	584	ARG	CD-NE-CZ	6.89	134.05	124.40
1	A	368	LEU	N-CA-C	6.89	119.64	111.71
2	B	73	VAL	CA-C-N	6.89	126.86	119.28
2	B	73	VAL	C-N-CA	6.89	126.86	119.28
1	C	468	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	A	615	LYS	CA-C-O	-6.88	113.13	120.42
2	B	305	ALA	CA-C-O	-6.88	113.12	120.42
1	C	292	MET	N-CA-C	6.88	119.62	111.71
1	A	434	ALA	CA-C-O	-6.88	113.54	120.90
2	B	342	ARG	CA-C-N	6.87	127.61	119.98
2	B	342	ARG	C-N-CA	6.87	127.61	119.98
1	A	385	ASN	N-CA-CB	6.87	121.80	110.39
2	D	338	VAL	O-C-N	-6.87	113.99	122.57
2	D	513	VAL	N-CA-CB	6.86	120.88	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	PRO	CA-C-N	6.86	126.46	119.19
2	B	48	PRO	C-N-CA	6.86	126.46	119.19
2	B	243	ASN	O-C-N	-6.86	114.39	122.20
2	B	266	LEU	CA-C-N	6.85	129.32	120.56
2	B	266	LEU	C-N-CA	6.85	129.32	120.56
1	C	314	GLN	CA-C-N	6.83	134.74	122.38
1	C	314	GLN	C-N-CA	6.83	134.74	122.38
1	A	232	MET	CA-C-N	6.83	126.79	119.28
1	A	232	MET	C-N-CA	6.83	126.79	119.28
1	A	385	ASN	CA-CB-CG	6.83	119.43	112.60
2	D	381	ASN	OD1-CG-ND2	-6.83	115.78	122.60
2	B	132	GLY	N-CA-C	6.81	124.72	115.32
1	A	150	ARG	CA-C-N	6.81	129.73	120.54
1	A	150	ARG	C-N-CA	6.81	129.73	120.54
2	B	115	ASP	CA-C-O	6.81	126.23	119.49
2	B	212	PRO	N-CA-CB	6.81	109.23	103.17
1	C	206	VAL	CA-CB-CG1	6.80	121.96	110.40
2	D	59	LEU	CA-C-N	6.80	129.72	120.54
2	D	59	LEU	C-N-CA	6.80	129.72	120.54
1	A	564	ARG	CA-CB-CG	6.80	127.70	114.10
2	B	224	LEU	CA-C-N	6.80	130.07	120.28
2	B	224	LEU	C-N-CA	6.80	130.07	120.28
1	A	333	GLY	O-C-N	-6.79	114.88	122.28
1	C	526	ASP	CA-C-N	6.79	126.75	119.28
1	C	526	ASP	C-N-CA	6.79	126.75	119.28
2	D	90	VAL	N-CA-CB	6.78	122.42	111.23
1	C	590	PHE	CA-CB-CG	6.78	120.58	113.80
1	C	182	ALA	O-C-N	-6.78	114.94	122.12
2	D	146	ALA	CA-C-N	6.78	127.05	119.32
2	D	146	ALA	C-N-CA	6.78	127.05	119.32
1	A	335	SER	CA-C-O	-6.77	111.05	119.38
1	A	673	ASP	O-C-N	-6.77	114.94	122.12
1	A	296	MET	CA-C-O	-6.76	113.38	120.55
1	A	673	ASP	CA-C-N	6.76	131.41	120.60
1	A	673	ASP	C-N-CA	6.76	131.41	120.60
2	B	500	LEU	CA-C-N	6.76	129.66	120.54
2	B	500	LEU	C-N-CA	6.76	129.66	120.54
1	C	72	HIS	CA-CB-CG	-6.76	107.04	113.80
1	A	597	ARG	CD-NE-CZ	6.75	133.85	124.40
1	C	129	ASN	CA-C-O	6.75	126.55	119.80
2	B	100	ARG	CD-NE-CZ	6.75	133.84	124.40
2	B	453	LEU	CA-C-N	6.74	129.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	453	LEU	C-N-CA	6.74	129.31	120.28
1	C	255	GLU	CA-C-N	6.74	129.55	120.65
1	C	255	GLU	C-N-CA	6.74	129.55	120.65
1	C	714	SER	CA-C-N	6.73	129.18	120.44
1	C	714	SER	C-N-CA	6.73	129.18	120.44
1	A	123	ARG	CA-C-N	6.72	133.37	120.66
1	A	123	ARG	C-N-CA	6.72	133.37	120.66
1	A	692	ASP	CA-CB-CG	6.72	119.32	112.60
2	D	586	LYS	CA-C-N	6.72	134.68	121.58
2	D	586	LYS	C-N-CA	6.72	134.68	121.58
1	C	134	GLY	CA-C-O	-6.71	113.60	120.45
1	C	5	PRO	N-CA-CB	6.71	109.23	103.19
2	B	61	ARG	NE-CZ-NH2	-6.71	113.17	119.20
2	B	398	PRO	N-CA-CB	6.71	110.63	103.39
2	D	478	PRO	N-CA-CB	6.70	109.28	103.31
1	A	221	ILE	CA-C-N	6.70	129.58	120.54
1	A	221	ILE	C-N-CA	6.70	129.58	120.54
2	B	459	PRO	N-CA-CB	6.70	110.41	103.38
2	B	123	LYS	CA-C-N	6.69	129.79	120.29
2	B	123	LYS	C-N-CA	6.69	129.79	120.29
1	A	63	THR	O-C-N	-6.68	114.48	123.10
1	A	612	ARG	CD-NE-CZ	6.68	133.75	124.40
1	A	664	LEU	N-CA-C	6.68	118.64	111.36
1	C	28	LEU	N-CA-C	6.68	118.56	111.28
2	D	309	GLU	O-C-N	-6.68	114.54	122.15
1	C	442	PRO	N-CA-CB	6.67	110.37	103.23
1	A	52	GLU	CA-C-N	6.66	130.44	120.31
1	A	52	GLU	C-N-CA	6.66	130.44	120.31
2	D	222	ARG	N-CA-C	6.66	119.39	111.33
2	D	267	VAL	CA-C-N	6.65	131.83	120.72
2	D	267	VAL	C-N-CA	6.65	131.83	120.72
1	A	129	ASN	CA-C-O	6.65	126.03	119.51
1	C	636	THR	CA-C-N	6.64	126.15	119.24
1	C	636	THR	C-N-CA	6.64	126.15	119.24
2	B	495	GLU	N-CA-C	6.64	118.52	111.28
1	C	666	PRO	N-CA-CB	6.64	110.88	103.44
1	C	277	VAL	CA-C-N	6.63	131.80	120.72
1	C	277	VAL	C-N-CA	6.63	131.80	120.72
2	B	415	ALA	O-C-N	-6.63	115.24	122.07
1	A	79	TYR	O-C-N	-6.63	112.75	122.43
1	C	528	ASP	CA-C-N	6.62	132.72	121.14
1	C	528	ASP	C-N-CA	6.62	132.72	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	622	ALA	O-C-N	-6.62	115.10	122.12
1	C	247	GLU	CA-C-N	6.62	134.36	122.38
1	C	247	GLU	C-N-CA	6.62	134.36	122.38
1	C	576	ASN	N-CA-C	6.62	121.63	107.67
2	D	322	GLN	CB-CG-CD	6.62	123.84	112.60
2	B	65	HIS	CA-CB-CG	6.61	120.41	113.80
2	D	320	ALA	CA-C-N	6.61	131.43	122.84
2	D	320	ALA	C-N-CA	6.61	131.43	122.84
1	C	28	LEU	CA-C-N	6.61	129.13	120.28
1	C	28	LEU	C-N-CA	6.61	129.13	120.28
1	A	182	ALA	CA-C-N	6.61	130.35	120.31
1	A	182	ALA	C-N-CA	6.61	130.35	120.31
2	D	200	ASP	CA-C-N	6.60	126.11	119.24
2	D	200	ASP	C-N-CA	6.60	126.11	119.24
2	B	411	SER	CA-C-N	6.60	129.66	120.29
2	B	411	SER	C-N-CA	6.60	129.66	120.29
1	C	320	PRO	O-C-N	-6.60	113.33	122.30
1	C	624	LEU	CA-C-N	6.59	133.17	122.69
1	C	624	LEU	C-N-CA	6.59	133.17	122.69
2	D	493	ASP	CA-CB-CG	6.59	119.19	112.60
2	D	532	SER	CA-C-N	6.59	126.53	119.28
2	D	532	SER	C-N-CA	6.59	126.53	119.28
2	B	417	TRP	CA-C-N	6.59	129.11	120.28
2	B	417	TRP	C-N-CA	6.59	129.11	120.28
1	C	706	THR	O-C-N	-6.59	116.40	121.14
2	D	104	MET	CA-C-N	6.59	135.39	122.61
2	D	104	MET	C-N-CA	6.59	135.39	122.61
2	D	420	PHE	CA-C-N	6.58	129.33	120.65
2	D	420	PHE	C-N-CA	6.58	129.33	120.65
1	A	228	THR	O-C-N	-6.58	114.53	122.22
2	B	115	ASP	CA-C-N	6.58	126.35	119.05
2	B	115	ASP	C-N-CA	6.58	126.35	119.05
1	C	629	ASP	CA-CB-CG	-6.58	106.03	112.60
1	C	413	THR	CA-C-N	6.57	128.99	120.44
1	C	413	THR	C-N-CA	6.57	128.99	120.44
2	D	26	ASP	O-C-N	-6.57	113.39	122.46
1	C	401	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	358	GLY	O-C-N	-6.57	114.16	122.70
1	C	690	GLU	CA-C-N	6.56	129.08	120.28
1	C	690	GLU	C-N-CA	6.56	129.08	120.28
1	C	126	ASP	O-C-N	-6.56	115.37	122.85
1	A	452	ARG	NE-CZ-NH2	-6.56	113.30	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	HIS	CA-CB-CG	6.56	120.36	113.80
1	A	683	THR	N-CA-CB	6.56	121.82	111.20
1	C	712	PRO	O-C-N	-6.55	113.77	122.22
2	D	432	ALA	N-CA-C	6.55	119.26	111.33
1	C	388	LEU	CA-C-N	6.55	128.96	120.44
1	C	388	LEU	C-N-CA	6.55	128.96	120.44
1	A	319	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	A	426	GLU	CB-CG-CD	6.54	123.72	112.60
1	A	127	SER	CA-C-O	6.54	127.42	119.38
1	A	661	HIS	CA-C-O	-6.53	113.91	120.90
1	C	189	PRO	O-C-N	-6.53	114.73	122.24
1	C	86	ILE	CA-C-N	-6.53	113.19	123.24
1	C	86	ILE	C-N-CA	-6.53	113.19	123.24
1	C	333	GLY	O-C-N	-6.53	115.17	122.28
1	A	117	PHE	CA-CB-CG	6.52	120.32	113.80
2	B	151	ASP	CA-C-N	6.52	128.91	120.44
2	B	151	ASP	C-N-CA	6.52	128.91	120.44
1	A	327	THR	N-CA-C	6.51	119.79	109.50
1	C	333	GLY	CA-C-N	6.51	129.66	120.28
1	C	333	GLY	C-N-CA	6.51	129.66	120.28
1	A	578	PRO	CA-C-N	6.51	129.53	120.29
1	A	578	PRO	C-N-CA	6.51	129.53	120.29
1	A	61	LEU	N-CA-C	6.50	120.32	112.38
1	A	711	ILE	CA-C-O	6.50	123.05	118.69
1	C	615	LYS	CA-C-O	-6.50	113.53	120.42
1	A	598	PRO	N-CA-CB	6.50	109.12	103.27
1	C	710	VAL	CA-C-N	6.49	125.52	120.33
1	C	710	VAL	C-N-CA	6.49	125.52	120.33
1	A	693	PHE	CA-CB-CG	6.49	120.29	113.80
2	D	60	LYS	CA-C-N	6.48	130.17	120.31
2	D	60	LYS	C-N-CA	6.48	130.17	120.31
2	B	251	GLU	CB-CG-CD	6.48	123.62	112.60
2	B	407	SER	O-C-N	-6.48	115.25	122.12
1	A	383	ALA	CA-C-N	6.48	129.49	120.29
1	A	383	ALA	C-N-CA	6.48	129.49	120.29
2	B	492	ARG	CA-C-N	6.48	130.16	120.31
2	B	492	ARG	C-N-CA	6.48	130.16	120.31
2	B	531	SER	N-CA-C	6.48	118.42	111.36
1	A	213	PRO	CA-C-N	6.47	125.97	119.24
1	A	213	PRO	C-N-CA	6.47	125.97	119.24
1	C	271	GLU	O-C-N	-6.47	115.26	122.12
1	C	41	ALA	CA-C-N	6.47	134.00	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	ALA	C-N-CA	6.47	134.00	121.18
1	A	493	LYS	CA-C-N	6.47	132.46	121.14
1	A	493	LYS	C-N-CA	6.47	132.46	121.14
1	C	677	ARG	CA-C-N	6.47	126.17	119.64
1	C	677	ARG	C-N-CA	6.47	126.17	119.64
1	A	281	ALA	O-C-N	-6.46	114.64	120.71
2	D	449	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	282	PRO	CA-C-N	6.46	132.44	121.14
1	A	282	PRO	C-N-CA	6.46	132.44	121.14
1	A	588	GLU	O-C-N	-6.45	115.28	122.12
1	C	651	VAL	CA-C-O	6.45	127.85	120.76
2	B	423	VAL	O-C-N	-6.44	115.50	121.94
2	D	336	PRO	CA-C-N	6.43	129.55	120.28
2	D	336	PRO	C-N-CA	6.43	129.55	120.28
1	C	597	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	A	149	MET	CA-C-N	6.42	129.72	120.79
1	A	149	MET	C-N-CA	6.42	129.72	120.79
1	A	175	LEU	CA-C-N	6.42	129.41	120.29
1	A	175	LEU	C-N-CA	6.42	129.41	120.29
1	C	80	ALA	CA-C-O	-6.42	113.74	120.55
1	A	401	ASP	CA-C-N	6.42	126.34	119.28
1	A	401	ASP	C-N-CA	6.42	126.34	119.28
2	D	375	PRO	O-C-N	-6.42	113.94	122.22
1	C	299	ALA	O-C-N	-6.42	115.32	122.12
1	C	188	LYS	CA-C-N	6.41	126.63	119.32
1	C	188	LYS	C-N-CA	6.41	126.63	119.32
1	C	243	TYR	CA-C-N	6.41	129.19	120.54
1	C	243	TYR	C-N-CA	6.41	129.19	120.54
1	A	288	TRP	CA-C-N	6.41	127.79	121.57
1	A	288	TRP	C-N-CA	6.41	127.79	121.57
2	B	328	TRP	CA-C-N	6.41	129.51	120.28
2	B	328	TRP	C-N-CA	6.41	129.51	120.28
1	C	487	THR	N-CA-C	6.41	118.27	111.28
2	D	298	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	C	370	GLU	N-CA-CB	-6.41	100.80	110.73
1	A	233	PRO	N-CA-CB	6.40	110.30	103.39
2	B	532	SER	CA-C-N	6.40	126.61	119.32
2	B	532	SER	C-N-CA	6.40	126.61	119.32
1	C	683	THR	N-CA-CB	6.40	122.02	111.08
2	D	141	ASP	CA-CB-CG	6.39	118.99	112.60
2	B	483	PRO	N-CA-CB	6.39	108.69	103.32
2	D	328	TRP	CA-C-N	6.39	128.84	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	328	TRP	C-N-CA	6.39	128.84	120.28
2	D	398	PRO	O-C-N	-6.39	113.98	122.22
1	A	390	LEU	CA-C-O	-6.38	113.78	120.55
1	C	92	PHE	O-C-N	-6.38	116.56	123.26
1	A	319	ASN	CA-C-N	6.38	125.95	119.19
1	A	319	ASN	C-N-CA	6.38	125.95	119.19
1	C	221	ILE	CA-C-N	6.38	130.39	120.82
1	C	221	ILE	C-N-CA	6.38	130.39	120.82
2	D	243	ASN	O-C-N	-6.38	114.43	122.27
1	C	388	LEU	CA-C-O	-6.37	113.80	120.55
2	D	498	GLU	CA-C-N	6.37	128.72	120.44
2	D	498	GLU	C-N-CA	6.37	128.72	120.44
2	B	264	ARG	NH1-CZ-NH2	6.37	127.58	119.30
1	A	135	ASP	CA-CB-CG	-6.37	106.23	112.60
1	A	318	LYS	N-CA-C	-6.37	106.05	113.88
1	C	220	ILE	CA-C-N	6.37	129.11	120.77
1	C	220	ILE	C-N-CA	6.37	129.11	120.77
2	D	495	GLU	N-CA-C	6.36	118.21	111.28
1	C	678	PRO	CA-C-N	6.36	128.80	120.28
1	C	678	PRO	C-N-CA	6.36	128.80	120.28
2	D	380	ARG	O-C-N	-6.36	114.45	122.27
1	C	515	ILE	CA-C-O	-6.36	114.43	121.17
2	B	266	LEU	N-CA-C	6.36	119.02	111.71
1	A	522	PRO	N-CA-CB	6.35	110.05	103.38
2	D	533	PRO	N-CA-CB	6.35	110.25	103.39
1	A	420	ALA	CA-C-N	6.33	129.09	120.54
1	A	420	ALA	C-N-CA	6.33	129.09	120.54
2	D	191	LYS	N-CA-C	6.33	120.26	112.54
1	A	690	GLU	O-C-N	-6.33	114.82	122.22
1	C	232	MET	CA-CB-CG	6.33	126.75	114.10
2	D	442	LEU	CA-C-N	6.33	129.27	120.29
2	D	442	LEU	C-N-CA	6.33	129.27	120.29
2	B	343	GLY	CA-C-N	6.32	128.66	120.44
2	B	343	GLY	C-N-CA	6.32	128.66	120.44
1	C	539	GLY	CA-C-N	6.32	129.04	120.38
1	C	539	GLY	C-N-CA	6.32	129.04	120.38
2	D	480	PRO	N-CA-CB	6.32	108.80	103.17
1	A	463	PRO	N-CA-CB	6.32	108.93	103.31
2	B	267	VAL	CA-C-N	6.31	128.74	120.28
2	B	267	VAL	C-N-CA	6.31	128.74	120.28
2	B	239	ASN	O-C-N	-6.31	115.43	122.12
1	C	526	ASP	O-C-N	-6.31	114.14	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ALA	CA-C-O	-6.30	114.21	120.82
2	B	275	GLU	CA-C-N	6.29	128.62	120.44
2	B	275	GLU	C-N-CA	6.29	128.62	120.44
1	A	524	ASP	CA-C-N	6.29	132.72	122.65
1	A	524	ASP	C-N-CA	6.29	132.72	122.65
1	A	401	ASP	O-C-N	-6.29	114.09	121.32
2	D	536	HIS	CA-C-N	6.29	128.71	120.60
2	D	536	HIS	C-N-CA	6.29	128.71	120.60
2	B	111	ALA	CA-C-N	6.29	130.79	122.30
2	B	111	ALA	C-N-CA	6.29	130.79	122.30
1	A	526	ASP	CA-C-N	6.28	125.91	119.56
1	A	526	ASP	C-N-CA	6.28	125.91	119.56
2	D	283	ARG	N-CA-CB	6.28	120.58	110.65
1	A	608	ASP	CA-CB-CG	6.28	118.88	112.60
2	D	365	GLN	N-CA-C	6.28	120.41	112.87
1	A	224	ILE	CA-C-O	-6.27	114.20	120.85
1	A	220	ILE	CA-C-N	6.27	128.98	120.77
1	A	220	ILE	C-N-CA	6.27	128.98	120.77
1	A	711	ILE	O-C-N	-6.27	116.41	120.42
1	A	132	VAL	O-C-N	-6.26	116.45	122.09
1	C	711	ILE	CA-C-O	6.26	122.88	118.69
1	A	129	ASN	CA-C-N	6.25	125.99	119.05
1	A	129	ASN	C-N-CA	6.25	125.99	119.05
2	D	365	GLN	CA-C-N	6.25	133.08	122.26
2	D	365	GLN	C-N-CA	6.25	133.08	122.26
1	A	442	PRO	N-CA-CB	6.25	109.96	103.15
1	A	483	VAL	N-CA-CB	6.25	118.12	111.00
2	B	24	ALA	O-C-N	-6.25	113.84	122.46
2	D	183	TYR	CA-C-N	6.25	129.81	120.31
2	D	183	TYR	C-N-CA	6.25	129.81	120.31
1	C	16	PRO	N-CA-CB	6.25	109.14	103.33
1	A	93	SER	N-CA-C	6.24	120.00	112.38
1	C	502	GLU	N-CA-C	6.24	118.16	111.36
1	C	343	ASN	CA-C-O	-6.24	111.94	119.49
2	B	536	HIS	CA-C-N	6.24	128.64	120.60
2	B	536	HIS	C-N-CA	6.24	128.64	120.60
1	A	526	ASP	CA-C-O	6.23	125.91	119.49
2	D	457	LYS	N-CA-C	-6.23	105.84	113.50
1	C	508	VAL	N-CA-CB	6.23	119.92	110.58
1	A	58	MET	CA-C-O	-6.22	113.95	121.05
1	A	358	GLY	CA-C-O	6.22	131.39	120.57
1	C	302	ARG	CD-NE-CZ	6.22	133.11	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	348	PHE	CA-C-N	6.21	128.61	120.28
2	B	348	PHE	C-N-CA	6.21	128.61	120.28
2	D	373	ASP	CA-CB-CG	6.21	118.81	112.60
2	D	306	ARG	CA-C-N	6.21	128.97	120.46
2	D	306	ARG	C-N-CA	6.21	128.97	120.46
2	B	456	ARG	CA-C-N	6.21	131.24	120.68
2	B	456	ARG	C-N-CA	6.21	131.24	120.68
2	B	82	PRO	N-CA-CB	6.21	109.22	103.39
1	C	222	SER	CB-CA-C	-6.21	100.44	110.74
2	D	362	PRO	N-CA-CB	6.20	108.83	103.31
1	A	382	ILE	CA-C-N	6.20	128.49	120.44
1	A	382	ILE	C-N-CA	6.20	128.49	120.44
1	A	457	ILE	O-C-N	-6.19	115.86	121.87
1	C	598	PRO	N-CA-CB	6.19	108.84	103.27
1	A	502	GLU	CB-CG-CD	6.18	123.11	112.60
1	C	538	ALA	CA-C-N	6.18	126.80	119.94
1	C	538	ALA	C-N-CA	6.18	126.80	119.94
1	C	660	GLY	O-C-N	-6.18	115.22	122.27
1	C	377	ASP	CA-C-N	6.18	128.56	120.28
1	C	377	ASP	C-N-CA	6.18	128.56	120.28
2	B	521	ARG	CA-C-N	6.18	131.18	120.68
2	B	521	ARG	C-N-CA	6.18	131.18	120.68
1	A	321	LYS	O-C-N	-6.17	114.37	122.39
2	D	177	GLU	CA-C-O	-6.17	114.30	120.90
1	A	350	ILE	O-C-N	-6.17	115.89	121.87
2	B	92	PRO	O-C-N	-6.17	109.38	121.10
1	A	674	LYS	O-C-N	-6.17	114.37	122.39
2	B	230	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	205	MET	O-C-N	-6.16	115.38	122.03
2	B	280	ILE	CA-C-N	6.16	132.26	122.59
2	B	280	ILE	C-N-CA	6.16	132.26	122.59
2	B	347	THR	CA-C-N	6.16	128.45	120.44
2	B	347	THR	C-N-CA	6.16	128.45	120.44
1	C	608	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	558	ARG	CD-NE-CZ	6.16	133.02	124.40
2	B	420	PHE	CA-C-N	6.15	128.53	120.28
2	B	420	PHE	C-N-CA	6.15	128.53	120.28
1	C	676	GLY	O-C-N	-6.15	115.14	122.34
2	B	191	LYS	N-CA-C	6.15	119.88	112.38
1	C	309	ALA	CA-C-N	6.15	128.43	120.44
1	C	309	ALA	C-N-CA	6.15	128.43	120.44
1	C	706	THR	CA-C-O	6.15	126.55	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	VAL	N-CA-C	6.15	117.63	110.62
1	C	132	VAL	CB-CA-C	-6.14	103.58	111.20
2	B	449	ARG	CD-NE-CZ	6.14	132.99	124.40
1	C	59	ASP	CA-CB-CG	6.14	118.74	112.60
2	D	141	ASP	CA-C-N	6.13	125.86	119.05
2	D	141	ASP	C-N-CA	6.13	125.86	119.05
1	A	295	PHE	CA-C-N	6.13	128.50	120.28
1	A	295	PHE	C-N-CA	6.13	128.50	120.28
1	A	436	ALA	O-C-N	-6.13	115.16	122.15
1	A	93	SER	CA-C-O	-6.13	112.08	119.49
1	C	214	PRO	O-C-N	-6.13	115.56	122.18
2	D	266	LEU	CA-C-N	6.13	128.86	120.46
2	D	266	LEU	C-N-CA	6.13	128.86	120.46
1	A	132	VAL	N-CA-C	6.12	118.05	112.29
2	D	77	ARG	CA-C-N	6.12	126.30	119.32
2	D	77	ARG	C-N-CA	6.12	126.30	119.32
1	C	381	ARG	CA-CB-CG	6.12	126.33	114.10
1	A	358	GLY	CA-C-N	6.11	133.22	121.54
1	A	358	GLY	C-N-CA	6.11	133.22	121.54
2	B	437	HIS	CA-CB-CG	-6.10	107.70	113.80
1	C	617	ILE	CA-C-O	-6.10	114.92	121.27
2	B	327	SER	N-CA-C	6.10	118.56	109.59
1	A	386	THR	CA-C-N	6.10	128.92	120.63
1	A	386	THR	C-N-CA	6.10	128.92	120.63
1	A	218	MET	CA-C-N	6.09	128.94	120.29
1	A	218	MET	C-N-CA	6.09	128.94	120.29
1	A	616	VAL	N-CA-CB	6.09	119.72	110.58
2	B	442	LEU	CA-C-N	6.09	128.44	120.28
2	B	442	LEU	C-N-CA	6.09	128.44	120.28
1	A	453	THR	CA-C-N	6.09	128.44	120.28
1	A	453	THR	C-N-CA	6.09	128.44	120.28
1	C	312	VAL	CA-C-N	6.08	129.04	120.28
1	C	312	VAL	C-N-CA	6.08	129.04	120.28
1	C	578	PRO	O-C-N	-6.08	115.61	122.18
1	A	79	TYR	CA-C-N	6.07	128.70	120.38
1	A	79	TYR	C-N-CA	6.07	128.70	120.38
1	A	445	ARG	CA-C-N	6.07	129.04	120.42
1	A	445	ARG	C-N-CA	6.07	129.04	120.42
1	A	466	GLY	O-C-N	-6.07	115.79	122.65
1	A	252	ALA	N-CA-C	6.07	118.69	111.71
1	A	120	PRO	N-CA-CB	6.07	110.00	103.33
1	A	146	ILE	N-CA-C	6.07	117.53	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	456	ARG	CA-C-O	6.06	126.97	120.55
1	C	327	THR	N-CA-C	6.06	119.08	109.50
2	D	189	PRO	N-CA-CB	6.06	108.58	103.25
1	C	634	PHE	CA-C-N	6.06	130.45	120.94
1	C	634	PHE	C-N-CA	6.06	130.45	120.94
2	B	352	VAL	O-C-N	-6.05	116.00	121.87
1	C	321	LYS	CA-C-N	6.05	128.88	120.29
1	C	321	LYS	C-N-CA	6.05	128.88	120.29
1	C	396	THR	N-CA-CB	6.05	119.44	110.49
2	D	339	ASN	CA-C-N	6.05	128.75	120.46
2	D	339	ASN	C-N-CA	6.05	128.75	120.46
1	A	718	LEU	CA-C-O	-6.05	114.47	120.70
2	D	94	THR	CA-C-O	-6.04	114.10	120.63
1	C	51	ASN	CA-C-N	6.04	130.26	120.60
1	C	51	ASN	C-N-CA	6.04	130.26	120.60
2	D	543	PRO	N-CA-CB	6.04	108.95	103.34
2	D	528	GLU	CA-C-N	6.03	127.88	120.22
2	D	528	GLU	C-N-CA	6.03	127.88	120.22
1	A	198	ASN	N-CA-C	6.03	119.96	112.24
1	C	314	GLN	O-C-N	-6.03	114.41	122.43
1	C	319	ASN	CA-C-N	6.03	125.65	119.56
1	C	319	ASN	C-N-CA	6.03	125.65	119.56
1	C	270	GLY	CA-C-N	6.02	128.35	120.28
1	C	270	GLY	C-N-CA	6.02	128.35	120.28
2	B	258	THR	CA-C-N	6.02	126.66	119.98
2	B	258	THR	C-N-CA	6.02	126.66	119.98
2	B	89	GLY	O-C-N	-6.01	114.89	122.41
1	A	80	ALA	CA-C-N	6.01	132.81	121.81
1	A	80	ALA	C-N-CA	6.01	132.81	121.81
1	A	232	MET	O-C-N	-6.01	116.36	121.23
2	B	141	ASP	CA-C-N	6.01	125.72	119.05
2	B	141	ASP	C-N-CA	6.01	125.72	119.05
1	C	103	ARG	CD-NE-CZ	6.01	132.81	124.40
2	D	119	LYS	CA-C-N	6.00	128.58	120.65
2	D	119	LYS	C-N-CA	6.00	128.58	120.65
1	A	243	TYR	O-C-N	-6.00	115.66	122.08
1	C	693	PHE	N-CA-C	6.00	117.82	111.28
1	A	216	PRO	O-C-N	-6.00	115.03	122.23
2	B	362	PRO	N-CA-CB	6.00	108.65	103.31
2	B	406	GLU	CB-CG-CD	6.00	122.80	112.60
1	A	170	ALA	CA-C-N	5.99	128.10	120.56
1	A	170	ALA	C-N-CA	5.99	128.10	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	GLU	N-CA-CB	5.99	119.10	110.06
1	C	240	ILE	CB-CG1-CD1	5.99	126.37	113.80
2	D	234	VAL	CA-C-O	5.99	126.83	120.48
2	D	605	ASP	CA-C-N	5.98	128.62	120.54
2	D	605	ASP	C-N-CA	5.98	128.62	120.54
1	C	450	ALA	CA-C-N	5.98	128.78	120.29
1	C	450	ALA	C-N-CA	5.98	128.78	120.29
1	A	392	GLN	CA-C-O	-5.98	112.84	120.31
1	C	612	ARG	CA-C-N	5.98	126.57	119.94
1	C	612	ARG	C-N-CA	5.98	126.57	119.94
1	A	420	ALA	N-CA-CB	5.97	119.00	110.16
2	B	201	PRO	CA-C-N	5.96	128.63	120.46
2	B	201	PRO	C-N-CA	5.96	128.63	120.46
1	C	43	GLN	CB-CG-CD	5.96	122.74	112.60
1	C	7	PHE	N-CA-C	5.96	120.17	113.02
1	C	198	ASN	CA-CB-CG	5.96	118.56	112.60
2	B	363	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	585	GLU	CA-C-N	5.95	128.25	120.28
1	A	585	GLU	C-N-CA	5.95	128.25	120.28
1	C	369	ASP	O-C-N	-5.95	114.76	122.37
2	B	337	TYR	O-C-N	-5.94	115.27	122.22
2	D	337	TYR	CA-C-N	5.94	132.66	121.97
2	D	337	TYR	C-N-CA	5.94	132.66	121.97
1	A	5	PRO	N-CA-CB	5.94	108.53	103.19
1	A	54	VAL	O-C-N	-5.94	115.87	121.87
1	C	350	ILE	O-C-N	-5.94	115.09	121.80
1	C	682	ILE	O-C-N	-5.94	116.94	123.18
2	D	405	VAL	CA-C-N	5.94	128.16	120.44
2	D	405	VAL	C-N-CA	5.94	128.16	120.44
2	B	90	VAL	O-C-N	-5.93	116.21	123.09
2	B	480	PRO	N-CA-CB	5.93	108.53	103.19
1	A	714	SER	CA-C-N	5.93	128.15	120.44
1	A	714	SER	C-N-CA	5.93	128.15	120.44
1	A	249	GLY	CA-C-O	-5.93	110.26	120.57
1	C	540	ARG	NE-CZ-NH1	-5.93	115.57	121.50
2	D	544	GLN	N-CA-C	5.93	116.10	108.34
1	A	645	VAL	O-C-N	-5.92	115.73	121.83
1	A	343	ASN	CA-C-N	5.92	129.31	120.31
1	A	343	ASN	C-N-CA	5.92	129.31	120.31
2	D	511	PRO	N-CA-CB	5.92	108.58	103.31
1	C	313	HIS	O-C-N	-5.91	115.30	122.22
2	D	32	GLU	CB-CG-CD	5.90	122.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	243	ASN	CA-C-N	5.89	132.85	121.18
2	B	243	ASN	C-N-CA	5.89	132.85	121.18
1	C	61	LEU	N-CA-C	5.89	119.57	112.38
2	D	364	THR	CA-C-N	5.89	131.95	120.99
2	D	364	THR	C-N-CA	5.89	131.95	120.99
1	C	556	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	377	ASP	CA-C-N	5.89	128.45	120.44
1	A	377	ASP	C-N-CA	5.89	128.45	120.44
1	A	688	ILE	CA-C-O	5.89	125.04	119.98
2	D	222	ARG	CA-C-N	5.89	129.26	120.31
2	D	222	ARG	C-N-CA	5.89	129.26	120.31
2	B	90	VAL	CB-CA-C	-5.88	100.42	111.30
1	C	131	ARG	CA-C-N	5.88	131.45	122.69
1	C	131	ARG	C-N-CA	5.88	131.45	122.69
1	C	586	LEU	CA-C-N	5.88	128.52	120.46
1	C	586	LEU	C-N-CA	5.88	128.52	120.46
1	A	458	ASP	CB-CG-OD1	5.88	131.92	118.40
1	A	252	ALA	CA-C-N	5.88	128.16	120.28
1	A	252	ALA	C-N-CA	5.88	128.16	120.28
2	D	423	VAL	O-C-N	-5.88	116.13	121.89
2	D	71	ASP	O-C-N	-5.88	116.52	123.22
1	A	189	PRO	N-CA-CB	5.87	109.79	103.33
1	C	436	ALA	CA-C-N	5.87	127.96	120.56
1	C	436	ALA	C-N-CA	5.87	127.96	120.56
2	D	238	ALA	O-C-N	-5.87	113.85	122.43
1	C	401	ASP	CA-C-N	5.87	125.74	119.28
1	C	401	ASP	C-N-CA	5.87	125.74	119.28
1	A	269	ALA	CA-C-N	5.87	127.73	120.34
1	A	269	ALA	C-N-CA	5.87	127.73	120.34
2	D	229	PRO	CA-C-N	5.87	132.04	122.65
2	D	229	PRO	C-N-CA	5.87	132.04	122.65
2	D	428	GLY	CA-C-O	-5.87	118.09	122.37
1	A	121	THR	O-C-N	-5.87	115.99	122.09
2	D	447	ALA	CA-C-O	-5.87	114.20	120.42
1	A	19	ALA	CA-C-N	5.86	131.91	123.17
1	A	19	ALA	C-N-CA	5.86	131.91	123.17
1	C	165	MET	CA-C-N	-5.86	114.14	122.41
1	C	165	MET	C-N-CA	-5.86	114.14	122.41
1	A	271	GLU	CA-C-N	5.86	130.50	120.72
1	A	271	GLU	C-N-CA	5.86	130.50	120.72
1	C	384	ARG	NH1-CZ-NH2	5.85	126.90	119.30
2	B	175	ALA	CA-C-N	5.85	128.44	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	ALA	C-N-CA	5.85	128.44	120.54
1	C	111	LYS	N-CA-C	5.85	117.65	111.28
2	D	610	GLU	CA-C-N	5.85	128.04	120.44
2	D	610	GLU	C-N-CA	5.85	128.04	120.44
1	A	420	ALA	CA-C-O	-5.84	114.23	120.42
1	A	222	SER	CA-C-O	-5.84	114.65	120.90
1	A	428	GLU	CA-C-N	5.84	128.11	120.28
1	A	428	GLU	C-N-CA	5.84	128.11	120.28
2	B	293	THR	CA-C-O	-5.84	114.69	120.82
1	C	205	MET	O-C-N	-5.83	115.79	122.09
1	A	10	VAL	N-CA-C	5.83	121.47	109.34
2	B	288	HIS	CA-CB-CG	5.83	119.63	113.80
1	A	706	THR	CA-C-O	5.82	126.26	121.08
2	B	495	GLU	O-C-N	-5.82	115.95	122.12
1	C	185	GLN	OE1-CD-NE2	-5.82	116.78	122.60
2	B	36	GLU	CA-C-N	5.81	130.43	120.72
2	B	36	GLU	C-N-CA	5.81	130.43	120.72
1	C	239	SER	CA-CB-OG	-5.81	99.48	111.10
1	C	181	THR	CA-C-N	5.81	128.34	120.38
1	C	181	THR	C-N-CA	5.81	128.34	120.38
1	A	438	GLU	CA-C-O	-5.81	113.54	120.10
1	A	114	SER	CB-CA-C	-5.80	99.69	109.50
2	B	361	LEU	CA-C-O	5.80	125.60	119.80
2	D	230	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	225	PHE	CA-C-N	5.80	127.98	120.44
1	A	225	PHE	C-N-CA	5.80	127.98	120.44
2	D	451	LYS	CA-C-N	5.80	128.37	120.54
2	D	451	LYS	C-N-CA	5.80	128.37	120.54
1	C	53	ASP	O-C-N	-5.80	114.66	122.43
2	D	127	GLU	CA-C-N	5.80	126.52	120.03
2	D	127	GLU	C-N-CA	5.80	126.52	120.03
2	D	363	PHE	CA-C-N	5.79	135.07	121.52
2	D	363	PHE	C-N-CA	5.79	135.07	121.52
1	C	427	VAL	O-C-N	-5.79	116.23	121.91
1	A	188	LYS	CA-C-N	5.79	125.48	119.05
1	A	188	LYS	C-N-CA	5.79	125.48	119.05
1	C	381	ARG	O-C-N	-5.79	114.70	122.23
1	A	610	HIS	CA-C-O	-5.79	114.04	120.70
1	C	54	VAL	O-C-N	-5.79	114.47	122.05
1	C	88	GLN	CA-C-O	-5.79	113.86	120.58
2	B	460	ILE	N-CA-CB	-5.79	104.82	112.34
2	D	492	ARG	CA-C-N	5.79	128.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	492	ARG	C-N-CA	5.79	128.61	120.28
1	C	520	GLY	CA-C-O	5.78	126.28	119.45
1	C	247	GLU	N-CA-C	5.78	119.15	111.75
1	C	298	VAL	CB-CA-C	-5.78	104.57	111.97
1	A	52	GLU	O-C-N	-5.78	113.17	122.41
1	A	677	ARG	CA-C-N	5.77	125.47	119.64
1	A	677	ARG	C-N-CA	5.77	125.47	119.64
2	B	73	VAL	O-C-N	-5.77	114.52	121.10
1	C	270	GLY	O-C-N	-5.77	116.59	122.19
1	A	281	ALA	CA-C-N	5.77	125.62	119.28
1	A	281	ALA	C-N-CA	5.77	125.62	119.28
1	C	349	CYS	CA-C-N	5.77	129.76	120.30
1	C	349	CYS	C-N-CA	5.77	129.76	120.30
1	A	291	GLY	CA-C-N	5.77	129.07	120.31
1	A	291	GLY	C-N-CA	5.77	129.07	120.31
1	C	524	ASP	CA-C-N	5.76	132.78	122.06
1	C	524	ASP	C-N-CA	5.76	132.78	122.06
1	A	724	ALA	CA-C-O	-5.76	114.41	120.63
2	B	365	GLN	O-C-N	-5.76	114.93	122.59
1	A	456	ARG	CD-NE-CZ	5.76	132.46	124.40
2	B	218	GLY	O-C-N	-5.76	116.14	122.24
1	C	665	VAL	CA-C-N	5.76	125.12	118.85
1	C	665	VAL	C-N-CA	5.76	125.12	118.85
2	D	116	PRO	N-CA-CB	5.76	109.39	103.23
1	C	221	ILE	CA-C-O	-5.75	115.42	121.41
2	B	90	VAL	CA-CB-CG2	5.75	120.18	110.40
1	A	18	PRO	N-CA-CB	5.75	108.35	103.35
1	C	674	LYS	CA-C-N	5.75	133.43	121.94
1	C	674	LYS	C-N-CA	5.75	133.43	121.94
1	A	694	ASP	CA-C-N	5.74	128.44	120.29
1	A	694	ASP	C-N-CA	5.74	128.44	120.29
1	C	443	LYS	CA-C-N	5.74	127.97	120.28
1	C	443	LYS	C-N-CA	5.74	127.97	120.28
2	D	348	PHE	CA-C-N	5.74	128.25	120.38
2	D	348	PHE	C-N-CA	5.74	128.25	120.38
1	A	344	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	616	VAL	CB-CA-C	-5.74	104.30	112.22
2	B	141	ASP	O-C-N	-5.74	114.72	121.32
1	C	151	GLU	CA-C-N	5.74	128.29	120.54
1	C	151	GLU	C-N-CA	5.74	128.29	120.54
2	B	320	ALA	CA-C-N	5.74	130.40	122.77
2	B	320	ALA	C-N-CA	5.74	130.40	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	275	GLU	CA-C-N	5.73	128.28	120.54
2	D	275	GLU	C-N-CA	5.73	128.28	120.54
2	B	310	VAL	O-C-N	-5.73	116.31	121.87
2	D	35	TRP	CA-C-N	5.73	128.28	120.54
2	D	35	TRP	C-N-CA	5.73	128.28	120.54
1	A	380	ALA	CA-C-O	-5.73	113.38	119.97
1	C	52	GLU	CA-C-N	5.73	130.29	120.72
1	C	52	GLU	C-N-CA	5.73	130.29	120.72
1	C	232	MET	CA-C-N	5.73	125.58	119.28
1	C	232	MET	C-N-CA	5.73	125.58	119.28
1	C	674	LYS	O-C-N	-5.73	114.55	122.46
1	A	622	ALA	O-C-N	-5.73	115.62	122.15
1	C	148	ASP	CA-C-N	5.72	128.41	120.29
1	C	148	ASP	C-N-CA	5.72	128.41	120.29
1	A	207	ARG	CA-C-O	5.72	126.40	119.31
1	A	247	GLU	O-C-N	-5.71	116.06	122.12
2	B	492	ARG	O-C-N	-5.71	116.28	122.79
2	D	105	ASP	CA-C-N	5.71	132.90	123.25
2	D	105	ASP	C-N-CA	5.71	132.90	123.25
2	B	370	PRO	N-CA-CB	5.71	108.28	103.25
2	B	243	ASN	CB-CG-ND2	5.71	124.96	116.40
1	C	122	HIS	O-C-N	-5.71	115.55	122.11
2	D	147	PRO	O-C-N	-5.70	115.68	122.24
1	C	400	ILE	CA-C-N	5.70	135.71	121.80
1	C	400	ILE	C-N-CA	5.70	135.71	121.80
2	D	483	PRO	N-CA-CB	5.70	108.39	103.31
1	C	438	GLU	O-C-N	-5.70	115.55	122.22
1	A	14	ASN	O-C-N	-5.70	114.82	122.22
2	B	71	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	504	ASP	CA-C-N	5.68	125.36	119.05
1	A	504	ASP	C-N-CA	5.68	125.36	119.05
2	D	91	ALA	CA-C-O	5.68	125.53	120.02
2	B	28	PRO	N-CA-CB	5.68	108.37	103.31
1	C	376	THR	CA-C-N	5.68	128.21	120.54
1	C	376	THR	C-N-CA	5.68	128.21	120.54
1	A	662	LEU	CA-C-O	-5.67	113.69	120.10
1	C	70	PHE	O-C-N	-5.67	115.77	122.58
1	A	388	LEU	CA-C-N	5.67	128.20	120.54
1	A	388	LEU	C-N-CA	5.67	128.20	120.54
2	D	563	GLN	CA-C-O	5.67	125.04	118.97
1	C	719	VAL	O-C-N	-5.67	116.35	121.91
1	A	293	ASN	CA-C-N	5.67	132.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASN	C-N-CA	5.67	132.37	121.54
1	A	41	ALA	O-C-N	-5.66	115.31	122.27
1	A	292	MET	N-CA-C	5.66	118.39	111.82
1	A	492	GLN	CA-C-N	5.66	128.33	120.29
1	A	492	GLN	C-N-CA	5.66	128.33	120.29
2	B	449	ARG	CA-C-N	5.66	127.87	120.28
2	B	449	ARG	C-N-CA	5.66	127.87	120.28
2	B	344	SER	O-C-N	-5.66	116.24	122.07
1	C	268	ARG	CA-C-N	5.65	127.86	120.28
1	C	268	ARG	C-N-CA	5.65	127.86	120.28
2	D	228	SER	CA-C-N	5.65	126.73	120.45
2	D	228	SER	C-N-CA	5.65	126.73	120.45
1	A	92	PHE	CA-C-O	5.65	127.37	121.38
1	C	10	VAL	N-CA-C	5.65	117.00	109.37
1	C	93	SER	CA-C-O	-5.65	113.71	120.10
2	B	341	LEU	CA-C-N	5.65	127.85	120.28
2	B	341	LEU	C-N-CA	5.65	127.85	120.28
2	B	358	ILE	CA-C-O	5.65	126.35	120.36
2	B	465	GLU	N-CA-CB	5.65	119.63	110.77
1	C	505	PRO	O-C-N	-5.65	115.02	122.64
1	C	196	ILE	O-C-N	-5.64	117.16	123.26
2	D	28	PRO	N-CA-CB	5.64	108.26	103.35
1	A	656	SER	CA-C-O	5.64	126.53	120.32
2	B	115	ASP	CA-CB-CG	5.64	118.24	112.60
2	D	259	GLY	CA-C-N	5.64	128.63	120.79
2	D	259	GLY	C-N-CA	5.64	128.63	120.79
1	A	689	PRO	CA-C-N	5.64	128.40	120.28
1	A	689	PRO	C-N-CA	5.64	128.40	120.28
2	D	218	GLY	N-CA-C	5.64	119.71	112.83
1	A	589	GLU	CA-C-N	5.64	128.09	120.65
1	A	589	GLU	C-N-CA	5.64	128.09	120.65
1	C	541	ALA	O-C-N	-5.64	113.39	122.41
1	C	564	ARG	CA-CB-CG	5.64	125.37	114.10
2	B	356	GLU	CB-CG-CD	5.63	122.18	112.60
1	C	678	PRO	N-CA-CB	5.63	108.70	103.46
1	A	197	GLN	CA-C-N	5.63	130.57	122.40
1	A	197	GLN	C-N-CA	5.63	130.57	122.40
1	A	397	THR	N-CA-C	-5.63	106.40	113.72
1	A	656	SER	O-C-N	-5.63	116.63	123.27
1	C	267	ILE	O-C-N	-5.63	116.41	121.87
2	B	164	VAL	N-CA-CB	5.63	119.73	111.52
1	A	454	GLN	CG-CD-NE2	5.62	124.84	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	VAL	CA-C-N	5.62	130.13	121.19
2	B	438	VAL	C-N-CA	5.62	130.13	121.19
2	D	479	PHE	CA-CB-CG	5.62	119.42	113.80
2	B	375	PRO	N-CA-CB	5.62	109.48	103.52
1	A	320	PRO	N-CA-CB	5.62	109.48	103.52
2	D	381	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	560	THR	N-CA-CB	5.62	119.38	110.84
2	D	467	PRO	CA-C-N	-5.62	115.07	122.99
2	D	467	PRO	C-N-CA	-5.62	115.07	122.99
1	A	290	ILE	N-CA-CB	5.62	119.46	111.82
2	D	79	LYS	O-C-N	-5.61	115.09	122.39
1	C	661	HIS	N-CA-C	5.61	118.16	111.71
1	A	340	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	469	LYS	CA-C-O	5.61	127.78	120.21
1	A	510	ALA	CA-C-N	5.60	127.73	120.44
1	A	510	ALA	C-N-CA	5.60	127.73	120.44
1	A	189	PRO	O-C-N	-5.60	115.51	122.23
1	A	432	GLY	CA-C-N	5.60	127.72	120.44
1	A	432	GLY	C-N-CA	5.60	127.72	120.44
2	B	376	LEU	CA-C-N	5.60	127.79	120.28
2	B	376	LEU	C-N-CA	5.60	127.79	120.28
1	A	328	HIS	CA-CB-CG	5.60	119.40	113.80
1	A	421	TRP	CA-C-N	5.60	127.33	120.22
1	A	421	TRP	C-N-CA	5.60	127.33	120.22
2	D	330	GLU	CA-C-O	-5.60	112.50	119.28
2	D	202	ILE	CA-C-N	5.60	126.15	119.94
2	D	202	ILE	C-N-CA	5.60	126.15	119.94
2	D	500	LEU	CA-C-N	5.59	130.08	121.19
2	D	500	LEU	C-N-CA	5.59	130.08	121.19
2	D	136	LEU	CA-C-O	5.59	127.43	121.11
2	D	584	ALA	CA-C-N	5.59	127.77	120.28
2	D	584	ALA	C-N-CA	5.59	127.77	120.28
1	C	306	MET	CA-C-N	5.59	127.77	120.28
1	C	306	MET	C-N-CA	5.59	127.77	120.28
1	C	123	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	C	293	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	141	VAL	CA-C-O	5.58	127.50	121.36
2	B	79	LYS	CA-C-N	5.58	132.49	122.38
2	B	79	LYS	C-N-CA	5.58	132.49	122.38
2	D	374	PHE	O-C-N	-5.58	114.91	121.32
2	D	85	LEU	CA-C-N	-5.58	109.88	122.04
2	D	85	LEU	C-N-CA	-5.58	109.88	122.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	ALA	CA-C-N	5.57	127.75	120.28
1	C	451	ALA	C-N-CA	5.57	127.75	120.28
1	A	662	LEU	N-CA-C	5.57	118.12	111.71
1	C	274	GLY	N-CA-C	5.57	122.16	114.92
1	C	166	THR	CB-CA-C	5.57	120.51	112.05
1	A	416	LEU	CA-C-N	5.57	127.68	120.44
1	A	416	LEU	C-N-CA	5.57	127.68	120.44
2	B	301	ARG	CA-C-O	-5.57	114.65	120.55
2	D	239	ASN	CA-C-N	5.56	131.98	121.97
2	D	239	ASN	C-N-CA	5.56	131.98	121.97
2	D	376	LEU	CA-C-N	5.56	127.67	120.44
2	D	376	LEU	C-N-CA	5.56	127.67	120.44
2	D	353	GLY	O-C-N	-5.56	116.42	122.54
1	A	256	MET	CA-CB-CG	5.56	125.21	114.10
2	B	25	GLY	CA-C-N	5.56	132.42	121.58
2	B	25	GLY	C-N-CA	5.56	132.42	121.58
1	A	307	LEU	CA-C-N	5.55	127.66	120.44
1	A	307	LEU	C-N-CA	5.55	127.66	120.44
2	B	95	ARG	N-CA-C	5.55	119.31	112.54
2	D	313	VAL	CA-C-O	-5.55	116.03	121.58
1	A	317	PRO	N-CA-CB	5.55	108.60	103.39
1	C	171	VAL	CA-C-O	-5.55	114.97	120.85
1	A	15	ALA	CA-C-O	5.54	127.75	120.16
1	C	568	GLY	CA-C-N	5.54	128.67	120.74
1	C	568	GLY	C-N-CA	5.54	128.67	120.74
2	B	314	ASP	CA-C-N	5.54	129.13	120.82
2	B	314	ASP	C-N-CA	5.54	129.13	120.82
2	B	235	THR	N-CA-CB	5.54	119.54	110.90
1	C	319	ASN	CB-CG-ND2	5.54	124.71	116.40
2	D	467	PRO	CA-C-O	-5.54	115.10	121.86
1	C	343	ASN	CA-CB-CG	5.54	118.14	112.60
1	C	313	HIS	CA-C-N	5.53	131.28	120.99
1	C	313	HIS	C-N-CA	5.53	131.28	120.99
1	C	224	ILE	N-CA-C	-5.53	105.14	110.72
2	B	477	LYS	CA-C-O	5.53	124.68	119.76
1	A	720	LYS	O-C-N	-5.52	115.85	122.15
1	C	58	MET	CA-C-O	-5.52	114.39	120.69
1	C	282	PRO	CA-C-N	5.52	132.34	121.58
1	C	282	PRO	C-N-CA	5.52	132.34	121.58
1	A	697	ARG	CA-C-N	5.52	128.69	120.31
1	A	697	ARG	C-N-CA	5.52	128.69	120.31
1	C	244	HIS	CA-CB-CG	-5.52	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	191	LYS	CA-C-N	5.51	132.35	122.38
2	B	191	LYS	C-N-CA	5.51	132.35	122.38
1	C	264	VAL	CA-C-N	5.51	127.66	120.28
1	C	264	VAL	C-N-CA	5.51	127.66	120.28
1	C	334	TRP	O-C-N	-5.51	115.78	122.22
1	A	400	ILE	O-C-N	-5.50	116.33	122.66
2	B	200	ASP	CA-C-O	5.50	127.70	120.16
1	C	246	GLN	O-C-N	-5.50	116.41	122.07
2	D	278	ASP	CA-C-N	5.50	130.18	121.44
2	D	278	ASP	C-N-CA	5.50	130.18	121.44
2	B	350	ALA	O-C-N	-5.49	116.41	122.07
1	C	428	GLU	O-C-N	-5.49	115.07	122.43
2	D	628	SER	CA-C-N	5.49	128.19	120.28
2	D	628	SER	C-N-CA	5.49	128.19	120.28
1	C	411	GLU	CA-C-O	-5.49	113.66	119.97
1	A	508	VAL	CB-CA-C	-5.49	104.65	112.22
2	D	600	LYS	N-CA-C	5.49	119.07	112.93
2	D	26	ASP	CA-C-N	5.48	135.38	123.15
2	D	26	ASP	C-N-CA	5.48	135.38	123.15
2	B	543	PRO	CA-C-O	-5.48	115.09	121.34
2	D	27	PHE	CA-C-O	5.48	126.95	120.87
2	B	25	GLY	O-C-N	-5.48	116.49	122.68
1	A	207	ARG	O-C-N	-5.47	114.91	122.46
1	A	693	PHE	N-CA-C	5.47	116.92	111.07
2	B	77	ARG	CA-C-O	5.47	127.65	120.16
2	B	147	PRO	O-C-N	-5.47	115.95	122.24
2	D	585	LEU	CA-C-N	5.47	127.61	120.28
2	D	585	LEU	C-N-CA	5.47	127.61	120.28
1	A	385	ASN	CA-C-N	5.46	127.92	120.54
1	A	385	ASN	C-N-CA	5.46	127.92	120.54
1	C	498	LYS	CA-C-N	5.46	127.86	120.38
1	C	498	LYS	C-N-CA	5.46	127.86	120.38
1	C	354	ALA	O-C-N	-5.46	116.44	122.07
1	C	645	VAL	CA-C-N	5.46	128.14	120.28
1	C	645	VAL	C-N-CA	5.46	128.14	120.28
2	B	23	LEU	O-C-N	-5.46	116.44	121.79
2	B	335	ASP	CA-C-N	5.46	125.07	119.56
2	B	335	ASP	C-N-CA	5.46	125.07	119.56
1	C	27	GLU	O-C-N	-5.45	116.45	122.07
2	D	37	ARG	CA-C-N	5.45	127.90	120.54
2	D	37	ARG	C-N-CA	5.45	127.90	120.54
1	C	376	THR	O-C-N	-5.45	116.52	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	610	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	255	GLU	CA-C-N	5.45	127.52	120.44
1	A	255	GLU	C-N-CA	5.45	127.52	120.44
1	C	697	ARG	O-C-N	-5.45	115.94	122.15
2	D	158	LEU	N-CA-C	-5.45	101.10	109.76
2	B	349	SER	CA-C-O	5.44	126.32	120.55
1	C	426	GLU	O-C-N	-5.44	116.47	122.07
2	B	566	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	625	GLY	N-CA-C	5.44	122.26	114.64
2	D	222	ARG	O-C-N	-5.44	116.35	122.12
1	A	40	THR	O-C-N	-5.44	115.08	122.36
1	C	456	ARG	CA-C-N	5.44	127.41	120.56
1	C	456	ARG	C-N-CA	5.44	127.41	120.56
1	A	146	ILE	CA-C-N	5.43	127.88	120.54
1	A	146	ILE	C-N-CA	5.43	127.88	120.54
1	A	179	VAL	O-C-N	-5.43	116.60	121.87
2	B	413	ALA	CA-C-N	5.43	127.50	120.44
2	B	413	ALA	C-N-CA	5.43	127.50	120.44
2	D	329	ARG	N-CA-C	5.43	117.20	111.28
2	D	363	PHE	O-C-N	-5.43	115.86	122.22
2	D	428	GLY	N-CA-C	-5.43	106.59	112.08
1	A	623	ASP	O-C-N	-5.43	115.59	122.27
1	C	201	LEU	O-C-N	-5.43	116.36	122.12
1	A	395	GLY	O-C-N	-5.43	115.59	122.32
1	C	522	PRO	N-CA-CB	5.43	108.14	103.36
2	D	309	GLU	CA-C-N	5.43	129.21	120.30
2	D	309	GLU	C-N-CA	5.43	129.21	120.30
2	D	338	VAL	CA-C-N	5.43	129.79	120.72
2	D	338	VAL	C-N-CA	5.43	129.79	120.72
2	D	471	ALA	CA-C-O	-5.43	115.04	120.96
1	C	326	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	C	505	PRO	N-CA-CB	5.42	108.94	103.25
2	B	491	HIS	CA-CB-CG	-5.42	108.38	113.80
2	B	459	PRO	CA-C-N	-5.42	114.71	122.84
2	B	459	PRO	C-N-CA	-5.42	114.71	122.84
1	C	710	VAL	CB-CA-C	5.42	118.19	111.15
2	B	404	TYR	O-C-N	-5.42	116.28	122.08
1	C	297	GLU	CA-C-O	-5.42	114.81	120.55
2	D	39	VAL	CA-C-N	5.42	128.94	120.82
2	D	39	VAL	C-N-CA	5.42	128.94	120.82
1	C	628	VAL	O-C-N	-5.42	117.49	123.18
2	D	288	HIS	CA-CB-CG	5.41	119.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	94	THR	CA-C-N	5.41	127.97	120.29
2	D	94	THR	C-N-CA	5.41	127.97	120.29
1	A	131	ARG	CA-C-N	5.41	129.96	122.28
1	A	131	ARG	C-N-CA	5.41	129.96	122.28
2	B	217	LEU	CA-C-N	5.41	126.90	120.14
2	B	217	LEU	C-N-CA	5.41	126.90	120.14
2	B	309	GLU	CA-C-N	5.41	127.87	120.46
2	B	309	GLU	C-N-CA	5.41	127.87	120.46
1	C	44	ILE	N-CA-C	-5.41	101.82	107.60
1	C	243	TYR	CA-C-O	5.41	126.68	121.00
1	C	87	ARG	CD-NE-CZ	5.40	131.96	124.40
2	D	439	THR	CA-C-N	5.40	127.52	120.28
2	D	439	THR	C-N-CA	5.40	127.52	120.28
1	A	430	VAL	O-C-N	-5.40	115.82	122.57
1	A	240	ILE	CB-CG1-CD1	5.40	125.14	113.80
2	D	413	ALA	CA-C-N	5.40	128.06	120.28
2	D	413	ALA	C-N-CA	5.40	128.06	120.28
2	B	78	PRO	N-CA-CB	5.40	109.41	103.26
1	C	263	GLY	CA-C-N	5.40	127.85	120.46
1	C	263	GLY	C-N-CA	5.40	127.85	120.46
1	C	434	ALA	CA-C-O	-5.39	114.83	120.55
2	D	74	PRO	CA-C-N	5.39	131.05	122.74
2	D	74	PRO	C-N-CA	5.39	131.05	122.74
1	A	639	GLU	N-CA-C	5.39	117.16	111.28
1	A	687	VAL	O-C-N	-5.38	116.38	122.36
1	C	350	ILE	CA-C-N	5.38	129.79	120.58
1	C	350	ILE	C-N-CA	5.38	129.79	120.58
2	D	297	LEU	N-CA-CB	5.38	119.17	110.40
1	A	20	ASP	O-C-N	-5.38	114.70	121.97
2	B	216	VAL	O-C-N	-5.38	115.88	122.12
1	A	70	PHE	O-C-N	-5.38	115.35	122.40
1	C	344	ASN	CA-C-N	5.38	127.34	120.56
1	C	344	ASN	C-N-CA	5.38	127.34	120.56
1	C	381	ARG	CB-CA-C	5.38	120.54	110.70
1	C	456	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	119	LEU	CA-C-N	5.38	125.02	119.05
1	A	119	LEU	C-N-CA	5.38	125.02	119.05
1	C	123	ARG	CA-C-N	5.38	132.02	121.06
1	C	123	ARG	C-N-CA	5.38	132.02	121.06
2	B	191	LYS	O-C-N	-5.37	115.40	122.39
1	A	69	PRO	CA-C-N	5.37	129.75	122.07
1	A	69	PRO	C-N-CA	5.37	129.75	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ALA	O-C-N	-5.37	116.42	122.12
2	B	273	ALA	CA-C-N	5.37	127.92	120.29
2	B	273	ALA	C-N-CA	5.37	127.92	120.29
2	D	212	PRO	N-CA-CB	5.37	108.89	103.25
2	D	262	TYR	N-CA-C	5.37	117.88	111.71
2	D	416	ALA	CA-C-N	5.37	127.74	120.44
2	D	416	ALA	C-N-CA	5.37	127.74	120.44
2	D	20	THR	N-CA-CB	5.37	119.85	111.64
1	A	486	SER	N-CA-C	5.36	122.22	110.80
2	B	304	TRP	CA-CB-CG	5.36	123.79	113.60
1	A	122	HIS	N-CA-C	5.36	117.54	111.11
1	A	426	GLU	CA-C-N	5.36	127.31	120.56
1	A	426	GLU	C-N-CA	5.36	127.31	120.56
1	C	44	ILE	O-C-N	5.36	125.85	120.92
2	B	306	ARG	CA-C-N	5.36	127.80	120.46
2	B	306	ARG	C-N-CA	5.36	127.80	120.46
2	B	340	ILE	CA-C-O	-5.36	115.49	121.17
1	A	556	PHE	N-CA-C	5.35	118.97	112.23
2	B	494	SER	CA-C-N	5.35	127.45	120.28
2	B	494	SER	C-N-CA	5.35	127.45	120.28
1	C	553	GLU	O-C-N	-5.35	116.45	122.12
1	C	129	ASN	CA-C-N	5.35	124.53	118.97
1	C	129	ASN	C-N-CA	5.35	124.53	118.97
1	C	183	GLU	CA-C-N	5.35	129.66	120.72
1	C	183	GLU	C-N-CA	5.35	129.66	120.72
2	D	154	LEU	N-CA-C	5.35	119.52	113.15
1	A	216	PRO	CA-C-N	5.35	127.45	120.28
1	A	216	PRO	C-N-CA	5.35	127.45	120.28
2	B	455	ASN	CA-C-O	5.35	125.82	119.56
1	A	214	PRO	N-CA-CB	5.35	108.98	103.15
2	D	252	LEU	O-C-N	-5.35	115.69	122.27
1	A	284	LEU	CA-C-N	5.35	131.11	122.29
1	A	284	LEU	C-N-CA	5.35	131.11	122.29
1	A	550	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	207	ARG	O-C-N	-5.34	115.14	122.46
2	D	408	LEU	O-C-N	-5.34	115.70	122.27
1	A	321	LYS	N-CA-C	5.34	118.90	112.38
2	D	557	PHE	CA-C-N	5.34	127.44	120.28
2	D	557	PHE	C-N-CA	5.34	127.44	120.28
2	B	77	ARG	O-C-N	-5.34	115.18	121.32
2	B	229	PRO	CA-C-N	5.34	131.19	122.65
2	B	229	PRO	C-N-CA	5.34	131.19	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	418	LYS	CA-C-N	5.34	127.44	120.28
2	B	418	LYS	C-N-CA	5.34	127.44	120.28
2	B	479	PHE	CA-C-O	5.34	124.78	119.49
1	C	134	GLY	N-CA-C	5.34	120.37	113.27
1	A	268	ARG	CA-C-O	-5.34	114.76	120.42
1	C	228	THR	CA-C-O	-5.34	112.81	119.38
1	A	16	PRO	N-CA-CB	5.33	108.29	103.33
2	D	362	PRO	O-C-N	-5.33	116.58	123.03
2	B	478	PRO	N-CA-CB	5.33	108.06	103.31
2	D	314	ASP	CA-C-N	5.33	127.74	120.54
2	D	314	ASP	C-N-CA	5.33	127.74	120.54
1	C	405	GLY	O-C-N	-5.33	115.77	122.70
1	A	476	PRO	N-CA-CB	5.33	108.25	103.08
1	C	417	ALA	CA-C-O	-5.33	115.22	120.82
1	A	712	PRO	O-C-N	-5.33	115.35	122.22
1	A	282	PRO	O-C-N	-5.32	115.35	122.22
1	C	603	ALA	CA-C-N	5.32	130.16	122.44
1	C	603	ALA	C-N-CA	5.32	130.16	122.44
2	B	128	GLY	O-C-N	-5.32	115.79	122.70
2	D	27	PHE	CA-CB-CG	-5.32	108.48	113.80
2	B	194	ALA	CA-C-O	5.32	126.22	120.32
2	B	579	LEU	CA-C-N	5.31	127.71	120.54
2	B	579	LEU	C-N-CA	5.31	127.71	120.54
1	A	73	GLY	CA-C-N	5.31	124.82	119.19
1	A	73	GLY	C-N-CA	5.31	124.82	119.19
1	A	193	ALA	CA-C-N	-5.31	113.58	120.91
1	A	193	ALA	C-N-CA	-5.31	113.58	120.91
2	B	333	ARG	CD-NE-CZ	5.31	131.83	124.40
2	B	374	PHE	O-C-N	-5.31	115.22	121.32
1	C	232	MET	O-C-N	-5.31	116.66	121.17
2	B	283	ARG	CD-NE-CZ	5.31	131.83	124.40
2	B	86	GLY	CA-C-N	5.30	135.68	122.74
2	B	86	GLY	C-N-CA	5.30	135.68	122.74
1	C	610	HIS	CA-C-O	-5.30	114.43	120.58
2	B	632	ASP	CA-C-N	5.30	128.01	120.53
2	B	632	ASP	C-N-CA	5.30	128.01	120.53
2	B	189	PRO	N-CA-CB	5.30	107.91	103.25
2	B	221	VAL	CA-C-N	5.30	127.69	120.54
2	B	221	VAL	C-N-CA	5.30	127.69	120.54
1	A	689	PRO	N-CA-CB	5.30	108.27	103.34
2	D	374	PHE	CA-C-N	5.29	125.11	119.28
2	D	374	PHE	C-N-CA	5.29	125.11	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	PHE	O-C-N	-5.29	116.51	122.12
1	C	560	THR	N-CA-CB	5.29	119.08	110.77
1	C	693	PHE	CA-C-N	5.29	127.37	120.28
1	C	693	PHE	C-N-CA	5.29	127.37	120.28
2	B	244	ALA	N-CA-C	5.29	119.36	113.01
2	B	441	VAL	CA-C-N	5.29	127.63	120.38
2	B	441	VAL	C-N-CA	5.29	127.63	120.38
2	B	543	PRO	N-CA-CB	5.29	108.02	103.31
1	C	553	GLU	CA-C-N	5.29	127.68	120.54
1	C	553	GLU	C-N-CA	5.29	127.68	120.54
2	B	49	PRO	N-CA-CB	5.28	109.12	103.52
2	B	406	GLU	CA-C-O	-5.28	115.27	120.82
2	B	398	PRO	CB-CA-C	-5.28	103.97	112.21
1	A	202	LYS	CA-C-N	5.28	127.30	120.44
1	A	202	LYS	C-N-CA	5.28	127.30	120.44
2	D	75	MET	CA-C-O	5.28	126.18	120.32
2	B	337	TYR	CA-C-N	5.28	131.47	121.97
2	B	337	TYR	C-N-CA	5.28	131.47	121.97
1	C	176	ALA	CB-CA-C	-5.28	102.03	110.79
1	A	591	GLU	O-C-N	-5.28	115.82	122.20
2	D	472	ARG	NH1-CZ-NH2	5.27	126.16	119.30
2	D	267	VAL	O-C-N	-5.27	116.76	121.87
1	A	583	ALA	CA-C-O	-5.27	114.94	120.63
1	C	499	LEU	CA-C-N	5.27	128.32	120.31
1	C	499	LEU	C-N-CA	5.27	128.32	120.31
1	A	297	GLU	CA-C-N	5.27	127.20	120.56
1	A	297	GLU	C-N-CA	5.27	127.20	120.56
1	C	475	GLU	CA-C-N	5.27	123.45	119.66
1	C	475	GLU	C-N-CA	5.27	123.45	119.66
1	C	636	THR	CA-C-O	5.27	129.20	121.46
2	D	217	LEU	CA-C-N	5.27	125.93	120.03
2	D	217	LEU	C-N-CA	5.27	125.93	120.03
2	B	59	LEU	CA-C-N	5.26	127.59	120.38
2	B	59	LEU	C-N-CA	5.26	127.59	120.38
1	C	82	ARG	CA-C-N	5.26	125.24	120.03
1	C	82	ARG	C-N-CA	5.26	125.24	120.03
2	B	333	ARG	N-CA-C	-5.26	106.55	113.12
1	C	231	ASN	N-CA-C	5.25	119.75	113.23
2	D	432	ALA	CA-C-N	5.25	128.96	120.55
2	D	432	ALA	C-N-CA	5.25	128.96	120.55
1	A	303	ALA	CA-C-N	5.25	127.32	120.28
1	A	303	ALA	C-N-CA	5.25	127.32	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	631	GLY	CA-C-N	5.25	125.19	119.78
1	C	631	GLY	C-N-CA	5.25	125.19	119.78
2	D	201	PRO	N-CA-CB	5.25	108.88	103.15
2	B	20	THR	O-C-N	-5.25	114.53	122.61
2	D	319	GLY	O-C-N	5.25	127.23	123.35
1	A	101	PHE	CA-C-O	-5.25	114.86	120.42
2	D	201	PRO	CA-C-N	5.25	127.17	120.56
2	D	201	PRO	C-N-CA	5.25	127.17	120.56
1	A	275	LEU	CA-C-N	-5.25	112.11	122.02
1	A	275	LEU	C-N-CA	-5.25	112.11	122.02
2	D	433	VAL	CA-C-N	5.25	127.31	120.28
2	D	433	VAL	C-N-CA	5.25	127.31	120.28
1	A	447	GLU	CA-C-N	5.25	127.26	120.44
1	A	447	GLU	C-N-CA	5.25	127.26	120.44
2	D	111	ALA	CA-C-N	5.25	129.38	122.30
2	D	111	ALA	C-N-CA	5.25	129.38	122.30
2	D	327	SER	CA-C-O	5.24	126.66	120.58
1	A	639	GLU	CA-C-N	5.24	127.73	120.29
1	A	639	GLU	C-N-CA	5.24	127.73	120.29
1	A	253	ASP	CA-C-N	5.24	127.27	120.56
1	A	253	ASP	C-N-CA	5.24	127.27	120.56
2	B	262	TYR	N-CA-C	5.24	118.93	112.54
2	B	448	GLU	O-C-N	-5.24	116.18	122.15
2	D	95	ARG	N-CA-C	5.24	117.07	111.36
1	A	44	ILE	CA-C-O	5.23	125.59	119.89
1	A	206	VAL	CB-CA-C	-5.23	102.71	111.29
2	D	315	GLU	N-CA-C	5.23	117.39	111.11
1	A	105	ASN	CA-CB-CG	-5.23	107.37	112.60
1	C	137	GLY	N-CA-C	5.23	122.49	115.59
1	C	457	ILE	CA-C-O	-5.22	115.63	121.17
1	C	588	GLU	O-C-N	-5.22	116.20	122.15
2	B	196	ASN	CA-CB-CG	5.22	117.82	112.60
2	B	521	ARG	CD-NE-CZ	5.22	131.71	124.40
1	A	641	ALA	CA-C-N	5.22	127.27	120.28
1	A	641	ALA	C-N-CA	5.22	127.27	120.28
2	D	421	GLN	CA-C-O	-5.22	115.52	121.00
2	B	442	LEU	N-CA-C	5.22	117.64	111.33
1	C	634	PHE	N-CA-C	5.22	119.22	112.86
2	B	382	THR	O-C-N	-5.21	116.70	122.07
2	B	455	ASN	O-C-N	-5.21	116.09	122.34
2	D	86	GLY	N-CA-C	-5.21	106.45	112.29
1	C	40	THR	O-C-N	-5.21	116.30	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ALA	CA-C-N	5.21	127.26	120.28
1	C	383	ALA	C-N-CA	5.21	127.26	120.28
1	C	459	SER	CA-CB-OG	-5.21	100.69	111.10
2	D	472	ARG	NE-CZ-NH2	-5.21	114.52	119.20
1	A	514	LYS	CA-CB-CG	5.20	124.51	114.10
1	C	268	ARG	CA-C-O	-5.20	115.03	120.55
2	D	142	PRO	N-CA-CB	5.20	109.05	103.33
1	C	243	TYR	O-C-N	-5.20	116.62	122.03
2	D	211	GLU	CA-C-N	5.20	126.34	119.84
2	D	211	GLU	C-N-CA	5.20	126.34	119.84
1	C	436	ALA	O-C-N	-5.20	115.36	122.33
1	C	693	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	218	MET	O-C-N	-5.19	116.15	122.22
2	D	219	ASP	CA-C-N	5.19	127.19	120.44
2	D	219	ASP	C-N-CA	5.19	127.19	120.44
2	D	465	GLU	CA-C-O	5.19	126.53	120.20
1	C	150	ARG	CA-C-N	5.19	128.01	120.79
1	C	150	ARG	C-N-CA	5.19	128.01	120.79
1	C	101	PHE	CA-CB-CG	5.19	118.99	113.80
1	C	665	VAL	O-C-N	-5.19	115.19	121.10
1	A	130	PRO	N-CA-CB	5.18	109.03	103.33
1	C	182	ALA	N-CA-C	5.18	117.60	111.33
2	B	458	GLN	CA-C-N	5.18	125.16	120.03
2	B	458	GLN	C-N-CA	5.18	125.16	120.03
2	D	147	PRO	N-CA-CB	5.18	109.16	103.26
1	A	695	GLU	CA-C-N	5.18	127.64	120.29
1	A	695	GLU	C-N-CA	5.18	127.64	120.29
1	A	723	ARG	CA-C-N	5.18	127.47	120.38
1	A	723	ARG	C-N-CA	5.18	127.47	120.38
1	C	158	LEU	CA-C-N	5.17	131.67	121.58
1	C	158	LEU	C-N-CA	5.17	131.67	121.58
2	D	88	PRO	N-CA-CB	5.17	108.15	103.34
1	A	451	ALA	CA-C-N	5.17	127.17	120.44
1	A	451	ALA	C-N-CA	5.17	127.17	120.44
1	C	249	GLY	O-C-N	5.17	129.23	121.83
1	C	87	ARG	CB-CA-C	5.17	119.48	112.09
1	C	213	PRO	N-CA-CB	5.17	108.09	103.08
1	C	264	VAL	O-C-N	-5.17	116.86	121.87
1	A	233	PRO	CB-CA-C	-5.17	104.15	112.21
1	A	249	GLY	CA-C-N	-5.17	113.37	120.71
1	A	249	GLY	C-N-CA	-5.17	113.37	120.71
2	D	242	HIS	N-CA-C	-5.17	105.73	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	GLU	O-C-N	-5.17	116.65	122.12
1	A	181	THR	CA-C-N	5.16	127.51	120.54
1	A	181	THR	C-N-CA	5.16	127.51	120.54
1	A	578	PRO	N-CA-CB	5.16	109.01	103.33
2	D	179	LEU	CA-C-O	-5.16	114.98	121.02
2	B	228	SER	CA-C-N	5.16	126.18	120.45
2	B	228	SER	C-N-CA	5.16	126.18	120.45
1	C	562	GLN	CB-CG-CD	-5.16	103.83	112.60
2	D	299	ALA	CA-C-O	-5.16	115.08	120.55
2	D	362	PRO	N-CA-C	-5.16	103.09	111.14
1	C	512	LEU	CA-C-N	5.16	127.71	120.28
1	C	512	LEU	C-N-CA	5.16	127.71	120.28
2	D	49	PRO	N-CA-CB	5.16	109.00	103.33
2	D	599	PHE	CA-C-N	5.15	131.20	122.65
2	D	599	PHE	C-N-CA	5.15	131.20	122.65
1	A	425	GLN	CA-C-N	5.15	127.14	120.44
1	A	425	GLN	C-N-CA	5.15	127.14	120.44
1	C	319	ASN	CA-C-O	5.15	123.88	119.66
1	C	552	LEU	CA-C-N	5.15	127.18	120.28
1	C	552	LEU	C-N-CA	5.15	127.18	120.28
2	D	609	ALA	CA-C-N	5.15	127.18	120.28
2	D	609	ALA	C-N-CA	5.15	127.18	120.28
1	A	65	ALA	O-C-N	-5.14	116.54	122.87
2	B	536	HIS	N-CA-C	5.14	118.66	112.38
1	C	225	PHE	CA-C-N	5.14	127.13	120.44
1	C	225	PHE	C-N-CA	5.14	127.13	120.44
1	C	606	GLY	O-C-N	-5.14	118.02	122.90
1	A	343	ASN	O-C-N	-5.14	115.71	122.39
2	B	386	LEU	CA-C-N	5.14	129.29	120.71
2	B	386	LEU	C-N-CA	5.14	129.29	120.71
1	C	200	ILE	CA-C-N	5.14	127.16	120.28
1	C	200	ILE	C-N-CA	5.14	127.16	120.28
2	D	352	VAL	CA-C-N	5.14	129.57	120.74
2	D	352	VAL	C-N-CA	5.14	129.57	120.74
2	B	456	ARG	NE-CZ-NH1	5.13	126.64	121.50
1	C	7	PHE	CA-C-N	5.13	128.11	120.31
1	C	7	PHE	C-N-CA	5.13	128.11	120.31
2	D	57	GLU	CA-C-N	5.13	127.11	120.44
2	D	57	GLU	C-N-CA	5.13	127.11	120.44
2	B	498	GLU	CA-C-N	5.13	127.15	120.28
2	B	498	GLU	C-N-CA	5.13	127.15	120.28
2	B	633	ILE	O-C-N	-5.13	116.86	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ASN	CA-CB-CG	5.12	117.72	112.60
2	B	142	PRO	N-CA-CB	5.12	108.96	103.33
2	D	121	THR	CA-C-O	-5.12	115.42	120.90
2	D	494	SER	CA-C-N	5.12	127.14	120.28
2	D	494	SER	C-N-CA	5.12	127.14	120.28
1	A	402	PRO	N-CA-CB	5.12	108.92	103.39
2	D	530	PHE	CA-CB-CG	-5.12	108.68	113.80
2	B	116	PRO	N-CA-CB	5.11	108.95	103.33
1	C	300	LYS	CA-C-N	5.11	128.08	120.31
1	C	300	LYS	C-N-CA	5.11	128.08	120.31
2	D	234	VAL	N-CA-C	5.11	115.33	108.17
2	D	150	LEU	CA-C-N	5.11	127.13	120.28
2	D	150	LEU	C-N-CA	5.11	127.13	120.28
1	C	384	ARG	CD-NE-CZ	5.11	131.55	124.40
2	D	26	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	318	ARG	NE-CZ-NH2	-5.11	114.61	119.20
2	B	530	PHE	CA-CB-CG	-5.11	108.69	113.80
2	B	311	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	122	HIS	CB-CA-C	-5.10	102.65	110.81
1	C	17	VAL	N-CA-C	-5.10	102.03	108.05
1	C	424	ILE	CA-C-N	5.10	127.11	120.28
1	C	424	ILE	C-N-CA	5.10	127.11	120.28
1	A	413	THR	CA-C-N	5.10	127.11	120.28
1	A	413	THR	C-N-CA	5.10	127.11	120.28
2	D	82	PRO	N-CA-CB	5.10	107.78	103.35
2	D	200	ASP	CA-C-O	5.10	127.14	120.16
1	C	308	TRP	CA-C-N	5.09	127.42	120.54
1	C	308	TRP	C-N-CA	5.09	127.42	120.54
2	D	336	PRO	N-CA-CB	5.09	108.89	103.39
1	C	73	GLY	CA-C-O	5.09	128.80	121.52
1	C	385	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	366	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	C	577	THR	CA-C-N	5.09	124.53	119.24
1	C	577	THR	C-N-CA	5.09	124.53	119.24
1	C	584	ARG	NE-CZ-NH1	5.09	126.59	121.50
2	D	263	VAL	N-CA-C	-5.08	105.75	110.53
1	C	518	ALA	CA-C-O	-5.08	114.12	119.97
1	A	66	GLY	CA-C-N	5.08	131.53	122.13
1	A	66	GLY	C-N-CA	5.08	131.53	122.13
2	B	350	ALA	CB-CA-C	5.08	118.86	110.88
1	C	231	ASN	O-C-N	-5.08	115.50	122.46
1	C	527	PRO	N-CA-CB	5.08	108.87	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	669	ARG	O-C-N	-5.07	116.61	122.09
2	B	542	THR	O-C-N	-5.07	116.81	121.37
1	C	296	MET	CA-C-N	5.07	127.07	120.28
1	C	296	MET	C-N-CA	5.07	127.07	120.28
2	D	129	LEU	CA-C-O	5.07	125.60	119.11
1	A	313	HIS	O-C-N	-5.07	115.47	122.46
1	A	460	GLY	CA-C-O	5.07	125.31	119.13
1	A	112	GLY	N-CA-C	5.07	117.29	111.36
2	B	172	GLN	CA-C-N	5.07	125.60	119.98
2	B	172	GLN	C-N-CA	5.07	125.60	119.98
1	A	140	GLY	CA-C-O	-5.07	116.03	121.35
1	C	233	PRO	N-CA-CB	5.07	108.86	103.39
2	B	364	THR	CA-C-N	5.06	131.21	121.54
2	B	364	THR	C-N-CA	5.06	131.21	121.54
1	C	138	MET	N-CA-C	5.06	116.61	111.14
1	A	434	ALA	O-C-N	-5.06	116.83	122.09
2	D	211	GLU	CB-CA-C	5.06	115.44	109.47
1	A	526	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	262	ASP	O-C-N	-5.06	116.83	122.09
2	B	39	VAL	CA-C-N	5.06	128.40	120.82
2	B	39	VAL	C-N-CA	5.06	128.40	120.82
1	C	120	PRO	N-CA-CB	5.06	108.89	103.33
2	B	238	ALA	O-C-N	-5.05	115.48	122.46
1	C	320	PRO	N-CA-CB	5.05	108.36	103.51
1	C	439	LYS	CA-C-N	5.05	130.12	121.07
1	C	439	LYS	C-N-CA	5.05	130.12	121.07
2	B	290	GLN	N-CA-C	5.05	116.47	111.07
2	B	336	PRO	CA-C-N	5.05	127.55	120.28
2	B	336	PRO	C-N-CA	5.05	127.55	120.28
1	A	505	PRO	N-CA-CB	5.05	108.88	103.33
2	D	551	ALA	CA-C-N	5.05	127.46	120.29
2	D	551	ALA	C-N-CA	5.05	127.46	120.29
2	B	204	PHE	O-C-N	-5.05	116.87	122.07
1	C	341	VAL	N-CA-C	5.05	119.10	112.04
1	C	646	GLU	CA-C-O	-5.05	114.40	120.10
1	A	250	ALA	CA-C-O	-5.04	115.64	121.19
1	A	513	ASP	N-CA-C	5.04	117.67	111.82
1	A	670	LYS	CA-C-O	-5.04	115.21	120.55
1	C	537	ASP	CA-C-O	-5.04	115.21	120.55
1	C	114	SER	CA-C-O	5.04	126.46	120.66
2	B	27	PHE	CA-C-O	5.04	126.73	120.54
1	C	79	TYR	CA-C-O	5.04	125.37	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	ILE	O-C-N	-5.04	116.64	121.83
1	C	290	ILE	CA-CB-CG1	5.03	118.95	110.40
1	C	343	ASN	CA-C-N	5.03	129.12	120.72
1	C	343	ASN	C-N-CA	5.03	129.12	120.72
2	D	104	MET	O-C-N	-5.03	115.58	122.33
1	A	707	PRO	N-CA-CB	5.03	107.68	103.25
2	D	106	ALA	CA-C-O	5.03	127.28	121.34
1	A	575	LYS	CA-C-O	-5.03	113.31	120.51
2	B	504	SER	CA-C-O	-5.03	114.57	120.20
2	B	555	GLU	CA-C-N	5.03	126.98	120.44
2	B	555	GLU	C-N-CA	5.03	126.98	120.44
1	A	4	LEU	CA-C-N	5.03	125.31	119.93
1	A	4	LEU	C-N-CA	5.03	125.31	119.93
1	A	603	ALA	N-CA-C	5.03	118.26	110.17
2	B	322	GLN	OE1-CD-NE2	5.03	127.63	122.60
1	A	261	ALA	O-C-N	-5.02	116.42	122.15
1	C	167	MET	O-C-N	-5.02	117.53	123.41
1	A	374	LEU	CA-C-O	5.02	124.86	120.19
1	A	642	ARG	O-C-N	-5.02	116.80	122.12
2	B	308	GLY	CA-C-N	5.02	126.97	120.44
2	B	308	GLY	C-N-CA	5.02	126.97	120.44
2	D	386	LEU	CA-C-N	5.02	127.27	120.44
2	D	386	LEU	C-N-CA	5.02	127.27	120.44
1	A	320	PRO	CA-C-N	5.02	128.63	120.60
1	A	320	PRO	C-N-CA	5.02	128.63	120.60
1	A	619	THR	CA-C-O	-5.02	115.23	120.55
1	C	349	CYS	CA-C-O	-5.02	115.55	120.82
2	D	378	ILE	CA-C-N	5.02	126.96	120.44
2	D	378	ILE	C-N-CA	5.02	126.96	120.44
2	B	501	MET	CA-C-N	5.02	127.31	120.54
2	B	501	MET	C-N-CA	5.02	127.31	120.54
1	A	261	ALA	CA-C-N	5.01	127.27	120.65
1	A	261	ALA	C-N-CA	5.01	127.27	120.65
1	A	264	VAL	CA-C-N	5.01	127.00	120.28
1	A	264	VAL	C-N-CA	5.01	127.00	120.28
1	C	93	SER	N-CA-C	5.01	117.48	111.71
1	C	260	LEU	CA-C-N	5.01	127.41	120.29
1	C	260	LEU	C-N-CA	5.01	127.41	120.29
1	A	132	VAL	CA-C-N	5.01	131.11	121.54
1	A	132	VAL	C-N-CA	5.01	131.11	121.54
1	A	409	VAL	CA-C-O	-5.01	114.84	120.25
1	A	193	ALA	CA-C-O	5.01	125.89	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	PHE	N-CA-C	5.01	118.68	112.47
1	A	397	THR	N-CA-CB	5.01	118.01	110.65
1	C	426	GLU	CA-C-N	5.01	126.87	120.56
1	C	426	GLU	C-N-CA	5.01	126.87	120.56
2	B	525	GLY	CA-C-N	5.00	125.50	119.94
2	B	525	GLY	C-N-CA	5.00	125.50	119.94
1	A	17	VAL	N-CA-C	-5.00	102.15	108.05
1	A	98	SER	O-C-N	-5.00	116.82	122.12
1	A	148	ASP	CB-CA-C	-5.00	102.81	110.81
1	C	546	GLY	CA-C-N	5.00	126.98	120.28
1	C	546	GLY	C-N-CA	5.00	126.98	120.28
2	B	124	ALA	CA-C-N	5.00	126.86	120.56
2	B	124	ALA	C-N-CA	5.00	126.86	120.56
1	C	639	GLU	CG-CD-OE1	5.00	129.91	118.40
2	D	283	ARG	CD-NE-CZ	5.00	131.40	124.40
2	D	631	LEU	CA-C-O	-5.00	115.75	121.00

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Mainchain
1	A	167	MET	Mainchain
1	A	20	ASP	Mainchain
1	A	313	HIS	Mainchain
1	A	342	TYR	Mainchain
1	A	376	THR	Mainchain
1	A	387	GLN	Mainchain
1	A	40	THR	Mainchain
1	A	405	GLY	Mainchain
1	A	409	VAL	Mainchain
1	A	588	GLU	Mainchain
1	A	625	GLY	Mainchain
1	A	627	ASP	Mainchain
1	A	665	VAL	Mainchain
1	A	672	LEU	Mainchain
1	A	677	ARG	Mainchain
1	A	697	ARG	Mainchain
1	A	70	PHE	Mainchain
1	A	723	ARG	Mainchain
2	B	103	ASP	Mainchain
2	B	204	PHE	Mainchain

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Mol	Chain	Res	Type	Group
2	B	220	TRP	Mainchain
2	B	228	SER	Mainchain
2	B	231	SER	Mainchain
2	B	277	PHE	Mainchain
2	B	334	GLU	Mainchain
2	B	337	TYR	Mainchain
2	B	339	ASN	Mainchain
2	B	380	ARG	Mainchain
2	B	391	ASN	Mainchain
2	B	394	ARG	Mainchain
2	B	401	GLY	Mainchain
2	B	418	LYS	Mainchain
2	B	456	ARG	Mainchain
2	B	465	GLU	Mainchain
2	B	82	PRO	Mainchain
2	B	86	GLY	Mainchain
1	C	126	ASP	Mainchain
1	C	158	LEU	Mainchain
1	C	167	MET	Mainchain
1	C	172	LEU	Mainchain
1	C	205	MET	Mainchain
1	C	215	GLN	Mainchain
1	C	27	GLU	Mainchain
1	C	313	HIS	Mainchain
1	C	342	TYR	Mainchain
1	C	356	THR	Mainchain
1	C	381	ARG	Mainchain
1	C	387	GLN	Mainchain
1	C	394	SER	Mainchain
1	C	40	THR	Mainchain
1	C	405	GLY	Mainchain
1	C	526	ASP	Mainchain
1	C	633	LEU	Mainchain
1	C	665	VAL	Mainchain
1	C	674	LYS	Mainchain
1	C	677	ARG	Mainchain
1	C	70	PHE	Mainchain
1	C	712	PRO	Mainchain
1	C	723	ARG	Mainchain
2	D	231	SER	Mainchain
2	D	237	ASP	Mainchain
2	D	324	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	D	337	TYR	Mainchain
2	D	380	ARG	Mainchain
2	D	387	ALA	Mainchain
2	D	391	ASN	Mainchain
2	D	394	ARG	Mainchain
2	D	401	GLY	Mainchain
2	D	86	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5564	0	5472	47	0
1	C	5564	0	5472	51	0
2	B	4616	0	4428	50	0
2	D	4616	0	4428	51	0
3	A	31	0	11	1	0
3	C	31	0	11	1	0
4	A	91	0	88	19	0
4	C	91	0	88	11	0
5	A	206	0	0	1	0
5	B	112	0	0	0	0
5	C	201	0	0	0	0
5	D	117	0	0	0	0
All	All	21240	0	19998	216	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 5.

All (216) 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:800:B12:H362	4:A:800:B12:H351	1.22	1.11
4:C:800:B12:H362	4:C:800:B12:H351	1.17	1.09
4:A:800:B12:H531	4:A:800:B12:H552	1.09	1.09
4:A:800:B12:H552	4:A:800:B12:C53	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.21	0.88
4:C:800:B12:H362	4:C:800:B12:C35	2.02	0.88
4:A:800:B12:H351	4:A:800:B12:C36	2.04	0.87
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.24	0.85
4:C:800:B12:H351	4:C:800:B12:C36	1.96	0.85
4:A:800:B12:H531	4:A:800:B12:C55	2.01	0.84
4:A:800:B12:H362	4:A:800:B12:C35	2.05	0.83
4:A:800:B12:H312	4:A:800:B12:C25	2.11	0.81
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.30	0.78
4:A:800:B12:H312	4:A:800:B12:H253	1.65	0.77
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.70	0.74
4:C:800:B12:H552	4:C:800:B12:H531	1.67	0.74
1:C:165:MET:HE3	1:C:196:ILE:HD12	1.71	0.73
1:A:228:THR:HG22	1:A:232:MET:HE3	1.71	0.71
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.73	0.71
1:A:165:MET:HE3	1:A:196:ILE:HD12	1.72	0.69
2:B:281:ASN:ND2	2:B:323:ASN:HD21	1.92	0.68
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.75	0.67
1:C:247:GLU:HB3	4:C:800:B12:H532	1.77	0.67
2:D:402:SER:HB3	2:D:405:VAL:HB	1.77	0.66
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.78	0.66
2:D:391:ASN:ND2	2:D:394:ARG:HH21	1.94	0.65
4:A:800:B12:H353	4:A:800:B12:H302	1.78	0.65
1:A:662:LEU:HD21	1:A:692:ASP:HB3	1.78	0.65
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.45	0.65
2:D:391:ASN:HD21	2:D:394:ARG:HH21	1.46	0.63
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.81	0.61
1:C:706:THR:HB	1:C:707:PRO:CD	2.30	0.61
2:D:165:GLU:HB2	2:D:196:ASN:HB2	1.81	0.61
1:C:448:GLU:HG2	1:C:569:VAL:HG21	1.83	0.60
4:C:800:B12:H531	4:C:800:B12:C55	2.32	0.60
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.84	0.60
1:C:122:HIS:HA	1:C:167:MET:HE1	1.84	0.59
1:C:605:MET:HE3	1:C:664:LEU:HB3	1.86	0.58
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.52	0.57
2:D:237:ASP:HB3	2:D:240:ILE:HD12	1.85	0.57
1:A:359:HIS:CE1	1:A:401:ASP:H	2.23	0.57
1:A:247:GLU:HB3	4:A:800:B12:H532	1.85	0.57
1:C:706:THR:HB	1:C:707:PRO:HD2	1.86	0.57
4:A:800:B12:C25	4:A:800:B12:C31	2.82	0.56
1:A:196:ILE:HG22	1:A:235:TRP:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:THR:HB	1:C:578:PRO:HD2	1.88	0.56
1:C:129:ASN:HB3	1:C:132:VAL:HG22	1.87	0.56
2:B:165:GLU:HB2	2:B:196:ASN:HB2	1.88	0.56
1:C:250:ALA:HB2	1:C:446:ILE:HG12	1.88	0.55
1:A:214:PRO:HG2	1:A:438:GLU:HG3	1.89	0.55
1:C:206:VAL:HG11	1:C:245:MET:HA	1.89	0.54
4:C:800:B12:H601	4:C:800:B12:H262	1.89	0.54
1:A:172:LEU:HB2	1:A:173:PRO:HD3	1.90	0.54
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.90	0.54
2:B:201:PRO:HB2	2:B:214:LEU:HD12	1.91	0.53
1:C:650:HIS:HB3	1:C:722:LEU:HD11	1.90	0.53
2:D:77:ARG:HB3	2:D:78:PRO:HD2	1.89	0.53
2:D:518:LEU:HD11	2:D:581:VAL:HG11	1.90	0.53
2:D:166:VAL:HG13	2:D:179:LEU:HD22	1.88	0.53
1:A:441:ILE:HB	1:A:442:PRO:CD	2.38	0.53
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.91	0.53
1:C:599:ARG:HG2	1:C:649:VAL:HA	1.90	0.52
1:C:149:MET:HE3	1:C:153:PHE:HE2	1.72	0.52
1:C:357:GLN:NE2	2:D:290:GLN:HE22	2.02	0.52
2:B:568:CYS:O	2:B:569:SER:HB2	2.09	0.52
4:A:800:B12:O28	4:A:800:B12:H3	2.10	0.51
2:D:433:VAL:HG23	2:D:438:VAL:HG21	1.92	0.51
1:C:282:PRO:HB3	1:C:321:LYS:HD2	1.93	0.51
1:A:336:LEU:HD22	1:A:344:ASN:HB3	1.93	0.51
2:B:532:SER:HB2	2:B:533:PRO:HD3	1.92	0.51
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.93	0.51
1:C:441:ILE:HB	1:C:442:PRO:CD	2.39	0.51
2:D:108:ASP:HB3	2:D:357:SER:HA	1.93	0.50
2:D:212:PRO:HG2	2:D:430:SER:HB3	1.92	0.50
2:D:208:GLN:HB2	2:D:210:THR:HG23	1.94	0.50
2:B:518:LEU:HD21	2:B:581:VAL:HG21	1.94	0.50
1:A:602:LEU:HD13	1:A:618:ALA:HA	1.92	0.50
2:B:245:GLY:HA2	2:B:449:ARG:HH12	1.77	0.50
1:C:67:ILE:HG21	2:D:30:ALA:HB2	1.93	0.50
1:A:95:ALA:HB1	1:A:151:GLU:HG2	1.93	0.49
4:A:800:B12:C36	4:A:800:B12:C35	2.77	0.49
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.03	0.49
2:D:197:LEU:HD11	2:D:224:LEU:HD13	1.94	0.49
4:A:800:B12:H312	4:A:800:B12:H251	1.92	0.49
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.95	0.49
2:D:515:LEU:HB2	2:D:544:GLN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:LYS:HB2	1:C:191:GLN:NE2	2.28	0.49
1:A:240:ILE:HD11	1:A:284:LEU:HD22	1.94	0.49
1:C:118:ASP:HA	1:C:139:ALA:HB3	1.95	0.49
4:A:800:B12:H2B	4:A:800:B12:O7R	2.13	0.48
2:B:426:LEU:HD11	2:B:432:ALA:HB2	1.95	0.48
2:B:511:PRO:HB2	2:B:540:ILE:HG12	1.95	0.48
2:B:598:ALA:HA	2:B:616:ARG:HH11	1.77	0.48
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.96	0.48
2:B:331:LEU:HD13	2:B:365:GLN:HB3	1.96	0.48
1:C:240:ILE:HD11	1:C:284:LEU:HD22	1.96	0.48
1:C:474:HIS:O	1:C:475:GLU:C	2.57	0.48
1:A:706:THR:HB	1:A:707:PRO:CD	2.44	0.47
1:C:12:LEU:HD12	2:D:306:ARG:HG2	1.97	0.47
1:C:359:HIS:CE1	1:C:401:ASP:H	2.31	0.47
4:C:800:B12:C35	4:C:800:B12:C36	2.73	0.47
2:B:126:LEU:HD22	2:B:156:ASP:HB3	1.96	0.47
1:C:683:THR:HG22	1:C:703:GLU:HB2	1.97	0.47
1:A:4:LEU:HD21	2:B:267:VAL:HG11	1.97	0.47
1:A:129:ASN:HB3	1:A:132:VAL:HG22	1.97	0.47
1:A:632:PRO:HG2	1:A:635:GLN:HG3	1.97	0.47
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.97	0.47
1:C:256:MET:HE2	1:C:420:ALA:HB3	1.97	0.47
1:A:282:PRO:HB3	1:A:321:LYS:HD2	1.97	0.46
1:A:683:THR:HG22	1:A:703:GLU:HB2	1.98	0.46
4:A:800:B12:H492	4:A:800:B12:C47	2.46	0.46
1:A:448:GLU:HG2	1:A:569:VAL:HG21	1.98	0.46
1:A:390:LEU:HA	1:A:394:SER:HB3	1.98	0.46
1:C:632:PRO:HD2	1:C:643:GLN:HE22	1.80	0.45
2:D:232:ARG:HG3	2:D:281:ASN:ND2	2.30	0.45
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.98	0.45
3:C:801:COA:H8A	3:C:801:COA:O4A	2.15	0.45
2:D:274:THR:HA	2:D:313:VAL:HG13	1.97	0.45
1:A:600:ILE:HG13	1:A:651:VAL:HG13	1.98	0.45
2:B:114:GLU:HG2	2:B:139:ARG:HB2	1.98	0.45
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.97	0.45
1:C:686:GLY:O	1:C:707:PRO:HD3	2.17	0.45
1:A:541:ALA:O	1:A:542:MET:HB2	2.16	0.45
2:B:238:ALA:HB2	2:B:255:ALA:HB2	1.98	0.45
1:C:574:VAL:O	1:C:575:LYS:HB2	2.16	0.45
2:D:426:LEU:HD11	2:D:432:ALA:HB2	1.99	0.45
1:A:504:ASP:O	1:A:508:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLN:HB2	1:C:216:PRO:HD3	1.98	0.45
2:D:170:TYR:HA	2:D:208:GLN:NE2	2.32	0.45
2:D:257:ALA:HB1	2:D:423:VAL:HG11	1.99	0.45
1:C:251:THR:HG23	1:C:449:ALA:HB1	1.99	0.45
1:A:63:THR:HB	5:A:808:HOH:O	2.17	0.44
2:D:538:ALA:HB2	2:D:627:LEU:HD13	1.98	0.44
2:D:238:ALA:HB2	2:D:255:ALA:HB2	2.00	0.44
2:B:369:LEU:HB2	2:B:477:LYS:HB2	1.98	0.44
4:A:800:B12:H8	4:A:800:B12:O39	2.18	0.44
2:B:107:TRP:HH2	2:B:392:ILE:HD11	1.83	0.44
1:A:188:LYS:HB3	1:A:189:PRO:HD2	2.00	0.44
2:B:290:GLN:HE21	2:B:345:ILE:HD11	1.83	0.43
2:D:267:VAL:HA	2:D:271:PHE:O	2.19	0.43
1:A:336:LEU:HD11	1:A:366:ASN:HB3	2.00	0.43
1:A:480:VAL:HG21	1:A:689:PRO:HB3	1.99	0.43
2:B:170:TYR:HA	2:B:208:GLN:NE2	2.33	0.43
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.53	0.43
2:B:518:LEU:HD11	2:B:581:VAL:HG11	2.00	0.43
1:A:394:SER:O	2:B:289:ASP:HA	2.18	0.43
2:B:92:PRO:O	2:B:93:PHE:HB2	2.18	0.43
2:D:292:LEU:HD23	2:D:408:LEU:HD21	2.00	0.43
2:B:73:VAL:HB	2:B:74:PRO:HD2	2.00	0.43
2:B:80:ASP:HB3	2:B:407:SER:HB2	1.99	0.43
2:B:281:ASN:HD22	2:B:323:ASN:ND2	2.00	0.43
2:B:592:ALA:HB2	2:B:633:ILE:HD13	2.01	0.43
1:C:586:LEU:HB3	1:C:719:VAL:HG11	2.00	0.43
1:A:706:THR:HB	1:A:707:PRO:HD2	2.01	0.43
1:A:54:VAL:O	1:A:58:MET:HE3	2.18	0.42
1:C:214:PRO:HG2	1:C:438:GLU:HG3	2.01	0.42
4:C:800:B12:H312	4:C:800:B12:H251	2.01	0.42
2:D:133:VAL:HG23	2:D:380:ARG:HD3	2.00	0.42
2:D:568:CYS:O	2:D:569:SER:HB2	2.18	0.42
1:A:399:VAL:O	1:A:402:PRO:HD3	2.19	0.42
1:C:167:MET:HE3	1:C:174:ILE:HG13	2.01	0.42
2:B:176:ALA:O	2:B:180:VAL:HG22	2.19	0.42
2:B:636:VAL:O	2:B:637:ALA:C	2.62	0.42
1:A:474:HIS:O	1:A:475:GLU:C	2.62	0.42
2:B:202:ILE:HG13	2:B:214:LEU:HD11	2.01	0.42
1:C:25:PHE:HB2	2:D:87:TYR:HB3	2.00	0.42
2:B:538:ALA:HB2	2:B:627:LEU:HD13	2.02	0.42
1:C:22:ALA:O	1:C:26:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:801:COA:H8A	3:A:801:COA:O4A	2.18	0.42
4:A:800:B12:O7R	4:A:800:B12:C2B	2.67	0.42
1:C:54:VAL:O	1:C:58:MET:HE3	2.20	0.42
1:C:441:ILE:N	1:C:442:PRO:HD2	2.35	0.42
4:C:800:B12:O39	4:C:800:B12:H8	2.19	0.42
1:A:4:LEU:HD13	2:B:264:ARG:HG2	2.01	0.42
1:A:472:LEU:HD21	2:B:377:ARG:NE	2.34	0.42
1:C:159:ASP:HB3	1:C:187:VAL:HG13	2.01	0.42
2:D:331:LEU:HD13	2:D:365:GLN:HB3	2.02	0.42
1:A:313:HIS:HB2	1:A:323:MET:SD	2.59	0.42
2:D:118:GLU:HG3	2:D:152:GLU:HG2	2.01	0.42
1:A:353:MET:HE3	2:B:290:GLN:NE2	2.35	0.42
2:D:564:VAL:HG13	2:D:592:ALA:HB3	2.02	0.41
2:B:334:GLU:O	2:B:335:ASP:C	2.63	0.41
1:C:200:ILE:HG12	1:C:217:SER:HB3	2.02	0.41
1:A:149:MET:HE2	1:A:178:TYR:HB2	2.02	0.41
1:C:652:VAL:HG11	1:C:668:LEU:HD21	2.03	0.41
2:B:200:ASP:N	2:B:201:PRO:HD3	2.36	0.41
2:D:103:ASP:HB3	2:D:105:ASP:OD1	2.20	0.41
2:D:517:CYS:HB2	2:D:545:VAL:O	2.20	0.41
1:A:665:VAL:N	1:A:666:PRO:HD2	2.36	0.41
1:C:249:GLY:HA3	1:C:450:ALA:HB2	2.02	0.41
2:D:390:VAL:HG12	2:D:392:ILE:HG23	2.02	0.41
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.99	0.41
1:A:256:MET:HE2	1:A:420:ALA:HB3	2.03	0.41
4:A:800:B12:H482	4:A:800:B12:H533	2.03	0.41
2:B:252:LEU:HD12	2:B:300:LEU:HD12	2.01	0.41
1:C:4:LEU:HD21	2:D:267:VAL:HG11	2.02	0.41
2:D:386:LEU:HD23	2:D:390:VAL:HG21	2.02	0.41
2:D:470:GLY:O	2:D:471:ALA:C	2.64	0.41
2:D:617:LEU:HD22	2:D:621:MET:HE1	2.03	0.41
1:A:171:VAL:HG11	1:A:198:ASN:ND2	2.36	0.41
2:B:554:VAL:HG21	2:B:584:ALA:HB1	2.03	0.41
4:C:800:B12:H312	4:C:800:B12:C25	2.51	0.41
1:C:459:SER:HA	1:C:577:THR:HG21	2.02	0.40
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.50	0.40
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.56	0.40
2:D:554:VAL:HG21	2:D:584:ALA:HB1	2.01	0.40
2:B:396:ASN:O	2:B:397:ASP:C	2.65	0.40
1:C:586:LEU:HD12	1:C:716:ILE:HG23	2.04	0.40
1:A:684:VAL:HG11	1:A:696:LEU:HD13	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:VAL:HB	2:B:636:VAL:HG13	2.02	0.40
2:B:537:ILE:HD13	2:B:623:VAL:HG21	2.02	0.40
1:C:28:LEU:HB3	2:D:99:VAL:HG21	2.03	0.40
1:A:550:ASP:O	1:A:554:LYS:HG2	2.21	0.40
2:B:102:GLY:O	2:B:394:ARG:HD3	2.22	0.40
1:A:652:VAL:HG11	1:A:668:LEU:HD21	2.03	0.40
2:D:190:ALA:O	2:D:227:PHE:HA	2.22	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	723/727 (99%)	682 (94%)	36 (5%)	5 (1%)	18	34
1	C	723/727 (99%)	688 (95%)	33 (5%)	2 (0%)	36	55
2	B	615/637 (96%)	569 (92%)	43 (7%)	3 (0%)	24	43
2	D	615/637 (96%)	576 (94%)	38 (6%)	1 (0%)	43	63
All	All	2676/2728 (98%)	2515 (94%)	150 (6%)	11 (0%)	30	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	SER
1	A	10	VAL
1	A	486	SER
1	A	542	MET
1	A	575	LYS
2	B	569	SER
1	C	475	GLU
2	D	508	SER

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Mol	Chain	Res	Type
1	A	475	GLU
2	B	508	SER
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	571/590 (97%)	540 (95%)	31 (5%)	20	41
1	C	571/590 (97%)	543 (95%)	28 (5%)	22	45
2	B	457/509 (90%)	438 (96%)	19 (4%)	26	52
2	D	457/509 (90%)	429 (94%)	28 (6%)	17	35
All	All	2056/2198 (94%)	1950 (95%)	106 (5%)	21	42

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	131	ARG
1	A	160	GLN
1	A	161	MET
1	A	198	ASN
1	A	202	LYS
1	A	234	LYS
1	A	239	SER
1	A	265	ASP
1	A	276	ASN
1	A	279	GLN
1	A	283	ARG
1	A	325	LEU
1	A	326	ARG
1	A	365	THR
1	A	370	GLU
1	A	381	ARG
1	A	406	SER

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Mol	Chain	Res	Type
1	A	454	GLN
1	A	482	LYS
1	A	483	VAL
1	A	493	LYS
1	A	498	LYS
1	A	503	ARG
1	A	533	LYS
1	A	562	GLN
1	A	564	ARG
1	A	574	VAL
1	A	602	LEU
1	A	651	VAL
1	A	725	SER
2	B	97	THR
2	B	148	GLU
2	B	150	LEU
2	B	163	LYS
2	B	199	LEU
2	B	222	ARG
2	B	226	LYS
2	B	230	ASP
2	B	279	THR
2	B	285	THR
2	B	297	LEU
2	B	300	LEU
2	B	433	VAL
2	B	460	ILE
2	B	508	SER
2	B	521	ARG
2	B	560	SER
2	B	612	LEU
2	B	617	LEU
1	C	9	SER
1	C	96	LYS
1	C	119	LEU
1	C	171	VAL
1	C	202	LYS
1	C	234	LYS
1	C	238	ILE
1	C	239	SER
1	C	241	SER
1	C	265	ASP

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Mol	Chain	Res	Type
1	C	276	ASN
1	C	279	GLN
1	C	283	ARG
1	C	325	LEU
1	C	370	GLU
1	C	381	ARG
1	C	482	LYS
1	C	483	VAL
1	C	508	VAL
1	C	533	LYS
1	C	562	GLN
1	C	574	VAL
1	C	594	GLU
1	C	597	ARG
1	C	602	LEU
1	C	629	ASP
1	C	651	VAL
1	C	688	ILE
2	D	57	GLU
2	D	67	VAL
2	D	140	VAL
2	D	141	ASP
2	D	148	GLU
2	D	150	LEU
2	D	163	LYS
2	D	199	LEU
2	D	211	GLU
2	D	226	LYS
2	D	228	SER
2	D	230	ASP
2	D	240	ILE
2	D	297	LEU
2	D	300	LEU
2	D	317	LYS
2	D	372	ASP
2	D	388	GLU
2	D	433	VAL
2	D	451	LYS
2	D	460	ILE
2	D	468	MET
2	D	508	SER
2	D	521	ARG

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Mol	Chain	Res	Type
2	D	564	VAL
2	D	567	LEU
2	D	569	SER
2	D	572	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	105	ASN
1	A	198	ASN
1	A	215	GLN
1	A	246	GLN
1	A	359	HIS
1	A	385	ASN
1	A	485	ASN
1	A	562	GLN
2	B	34	GLN
2	B	101	ASN
2	B	196	ASN
2	B	290	GLN
2	B	323	ASN
2	B	391	ASN
1	C	105	ASN
1	C	191	GLN
1	C	198	ASN
1	C	246	GLN
1	C	313	HIS
1	C	359	HIS
1	C	485	ASN
1	C	576	ASN
1	C	643	GLN
2	D	196	ASN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN
2	D	381	ASN
2	D	391	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	A	801	-	32,33,50	0.79	1 (3%)	50,52,75	0.79	1 (2%)
4	B12	A	800	1	94,101,101	1.03	4 (4%)	149,166,166	1.68	35 (23%)
4	B12	C	800	1	94,101,101	1.02	5 (5%)	149,166,166	1.63	31 (20%)
3	COA	C	801	-	32,33,50	0.76	0	50,52,75	0.87	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	801	-	-	6/21/37/64	0/3/3/3
4	B12	A	800	1	-	9/56/223/223	0/3/11/11
4	B12	C	800	1	-	5/56/223/223	0/3/11/11
3	COA	C	801	-	-	6/21/37/64	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	B12	C54-C17	2.98	1.59	1.54
4	C	800	B12	C54-C17	2.88	1.59	1.54
4	A	800	B12	C14-N23	2.78	1.38	1.35
4	A	800	B12	C46-C12	2.54	1.59	1.54
4	C	800	B12	C14-N23	2.46	1.38	1.35
4	A	800	B12	O6R-C1R	-2.37	1.36	1.42
4	C	800	B12	C19-N24	-2.32	1.46	1.49
4	C	800	B12	C48-C13	2.21	1.59	1.54
3	A	801	COA	P1A-O3A	2.09	1.61	1.59
4	C	800	B12	C46-C12	2.07	1.58	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	800	B12	C7-C6-C5	-5.60	119.32	128.07
4	C	800	B12	C2-C1-C19	-4.46	111.68	118.61
4	A	800	B12	C7-C6-C5	-4.36	121.26	128.07
4	A	800	B12	O58-C57-C56	-3.92	114.92	122.02
4	C	800	B12	C55-C17-C16	3.77	123.97	116.59
4	A	800	B12	C41-C8-C9	-3.71	104.71	111.19
4	A	800	B12	C2-C1-C19	-3.66	112.92	118.61
4	C	800	B12	C2-C1-N21	3.65	106.84	101.78
4	A	800	B12	C55-C17-C18	3.62	118.04	111.12
4	C	800	B12	O28-C27-N29	-3.62	112.85	122.53
4	C	800	B12	C25-C2-C1	3.55	119.06	113.75
4	C	800	B12	C20-C1-C2	3.55	119.14	113.28
4	C	800	B12	C1-C19-C18	-3.54	116.16	121.90
4	A	800	B12	C36-C7-C37	3.51	116.71	110.74
4	A	800	B12	C19-N24-C16	3.51	111.12	107.29
4	A	800	B12	C15-C16-N24	3.47	127.37	122.42
4	C	800	B12	C7-C6-N22	3.46	114.23	107.94
4	A	800	B12	C7-C6-N22	3.40	114.13	107.94
4	A	800	B12	O28-C27-N29	-3.30	113.72	122.53
4	C	800	B12	C2-C3-C4	3.29	105.35	101.64
4	A	800	B12	C26-C2-C3	-3.27	101.72	107.42
4	A	800	B12	C13-C14-N23	3.23	113.47	109.09
4	A	800	B12	C2P-C1P-N59	-3.22	108.19	112.92
4	C	800	B12	C48-C13-C12	-3.07	107.75	116.52
4	C	800	B12	C1P-N59-C57	-3.05	116.14	122.69
4	A	800	B12	C16-C15-C14	-3.05	116.61	121.26
4	A	800	B12	O51-C50-C49	-3.00	111.98	121.04
4	C	800	B12	C18-C19-N24	2.98	106.81	102.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	800	B12	C10-C9-N22	-2.82	122.52	125.74
4	A	800	B12	C18-C19-N24	2.82	106.57	102.33
4	A	800	B12	C46-C12-C11	-2.81	100.04	110.08
4	C	800	B12	C9-C10-C11	-2.77	122.01	125.97
4	A	800	B12	C17-C16-C15	-2.74	121.94	126.26
4	C	800	B12	C1-C2-C3	-2.65	98.26	101.60
4	A	800	B12	C49-C50-N52	2.58	124.77	116.49
4	C	800	B12	C19-C1-N21	-2.52	99.54	102.14
4	A	800	B12	C13-C12-C11	2.52	103.79	100.97
4	A	800	B12	C54-C17-C16	-2.51	99.40	112.41
4	C	800	B12	C13-C14-N23	2.49	112.46	109.09
4	A	800	B12	C13-C14-C15	-2.46	120.58	124.32
4	A	800	B12	C8B-N1B-C2B	2.45	108.49	106.26
4	A	800	B12	C4B-C5B-C6B	2.44	123.28	119.69
4	A	800	B12	C4B-C9B-C8B	-2.42	117.94	120.16
4	C	800	B12	C13-C14-C15	-2.39	120.68	124.32
4	C	800	B12	C30-C3-C2	-2.38	113.75	119.00
3	C	801	COA	O5A-P2A-O4A	2.35	120.00	110.83
4	C	800	B12	C36-C7-C37	2.28	114.62	110.74
3	A	801	COA	O5A-P2A-O4A	2.27	119.69	110.83
4	A	800	B12	C12-C13-C14	-2.27	98.53	102.26
4	A	800	B12	C26-C27-N29	2.27	123.52	116.49
4	A	800	B12	C3P-C2P-C1P	2.22	115.72	111.42
4	C	800	B12	C12-C11-C10	-2.20	120.56	123.40
4	A	800	B12	C35-C5-C4	2.20	121.25	116.79
4	C	800	B12	O44-C43-N45	-2.18	116.70	122.53
4	A	800	B12	C41-C8-C7	-2.18	108.19	114.19
4	A	800	B12	C55-C56-C57	-2.17	106.41	111.25
4	C	800	B12	C35-C5-C4	2.13	121.11	116.79
4	C	800	B12	C54-C17-C16	-2.13	101.36	112.41
4	A	800	B12	C48-C49-C50	-2.12	105.34	112.55
4	C	800	B12	O2-P-O3	-2.12	96.94	102.87
4	C	800	B12	C30-C31-C32	-2.12	105.35	112.55
4	C	800	B12	C19-N24-C16	2.08	109.57	107.29
4	C	800	B12	C35-C5-C6	-2.08	119.06	122.41
4	A	800	B12	C6-C5-C4	-2.04	117.91	121.55
4	C	800	B12	C1-C19-N24	-2.03	103.99	106.25
4	A	800	B12	C20-C1-C2	2.03	116.63	113.28
3	C	801	COA	C5A-N7A-C8A	2.03	106.63	103.45
4	C	800	B12	O34-C32-C31	-2.01	114.99	121.04
4	A	800	B12	C7B-C8B-C9B	2.00	124.87	122.47

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	B12	C16-C17-C55-C56
4	A	800	B12	C18-C17-C55-C56
4	A	800	B12	C2R-C1R-N1B-C2B
4	C	800	B12	C2R-C1R-N1B-C2B
3	A	801	COA	O4B-C4B-C5B-O5B
3	A	801	COA	C3B-C4B-C5B-O5B
4	A	800	B12	C2-C3-C30-C31
4	A	800	B12	C2R-C1R-N1B-C8B
4	C	800	B12	C2R-C1R-N1B-C8B
3	C	801	COA	O4B-C4B-C5B-O5B
3	C	801	COA	C3B-C4B-C5B-O5B
4	A	800	B12	O6R-C1R-N1B-C8B
4	C	800	B12	O6R-C1R-N1B-C8B
3	C	801	COA	P2A-O3A-P1A-O2A
4	A	800	B12	N59-C1P-C2P-O3
4	A	800	B12	N59-C1P-C2P-C3P
3	A	801	COA	P2A-O3A-P1A-O2A
3	A	801	COA	C3B-O3B-P3B-O7A
3	C	801	COA	C3B-O3B-P3B-O7A
3	A	801	COA	P2A-O3A-P1A-O1A
3	C	801	COA	P2A-O3A-P1A-O1A
4	C	800	B12	C2P-O3-P-O4
4	C	800	B12	C2P-O3-P-O5
3	C	801	COA	C3B-O3B-P3B-O8A
3	A	801	COA	C2B-C1B-N9A-C8A
4	A	800	B12	O6R-C1R-N1B-C2B

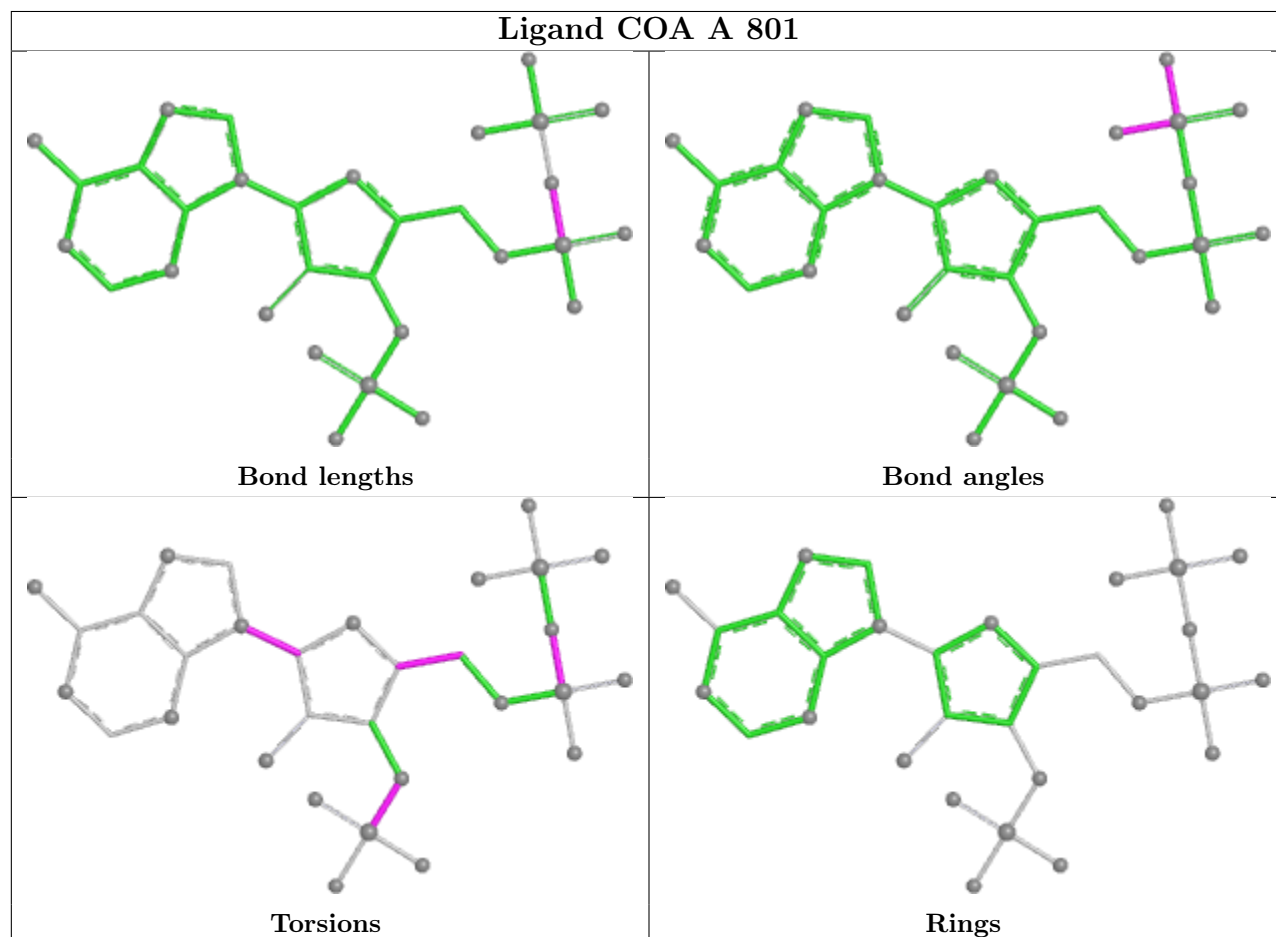
There are no ring outliers.

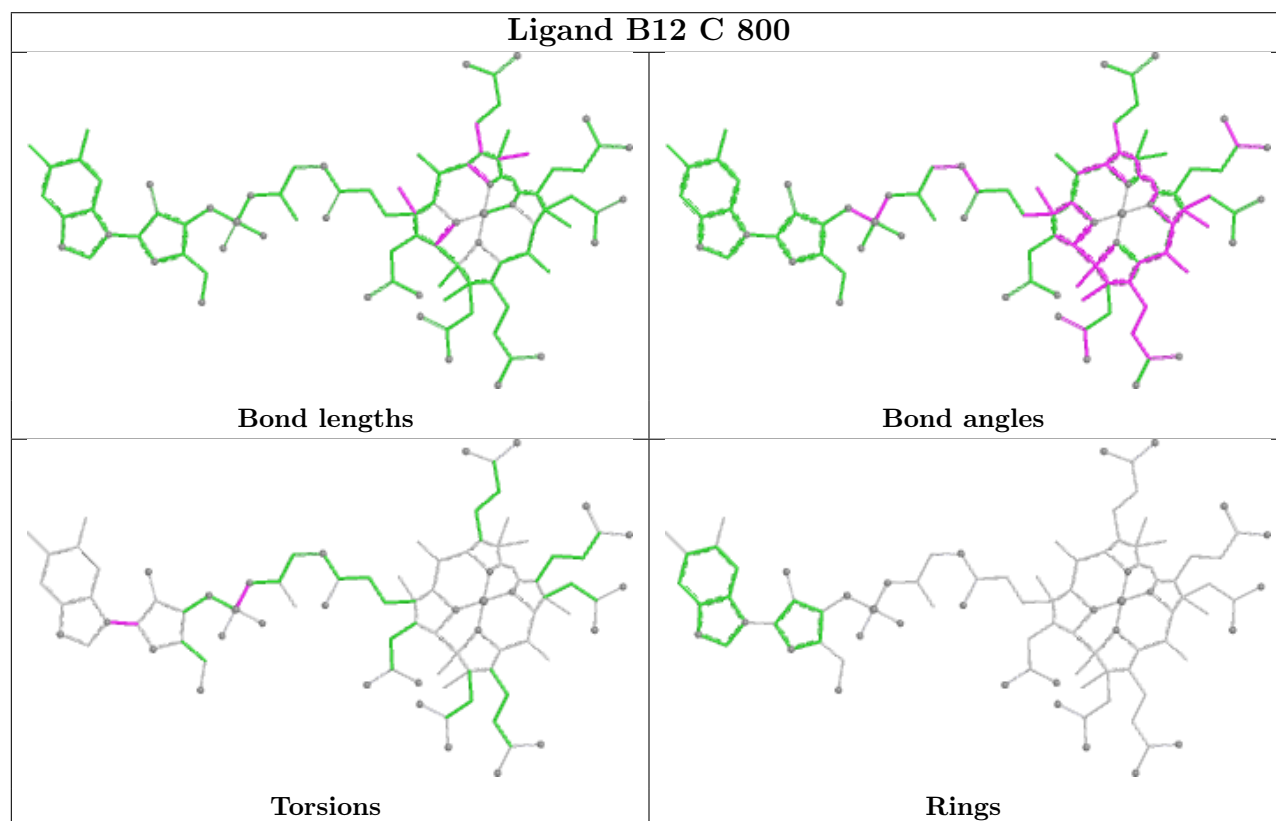
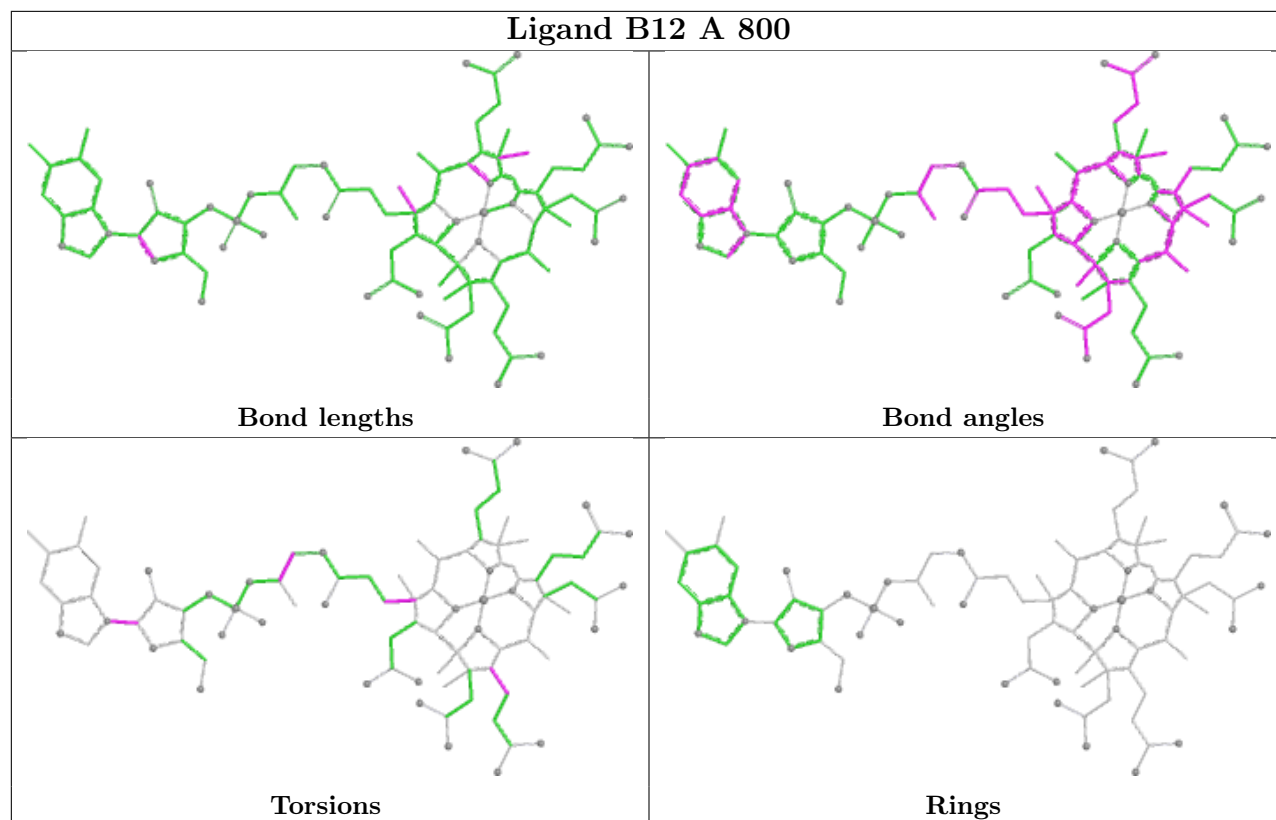
4 monomers are involved in 32 short contacts:

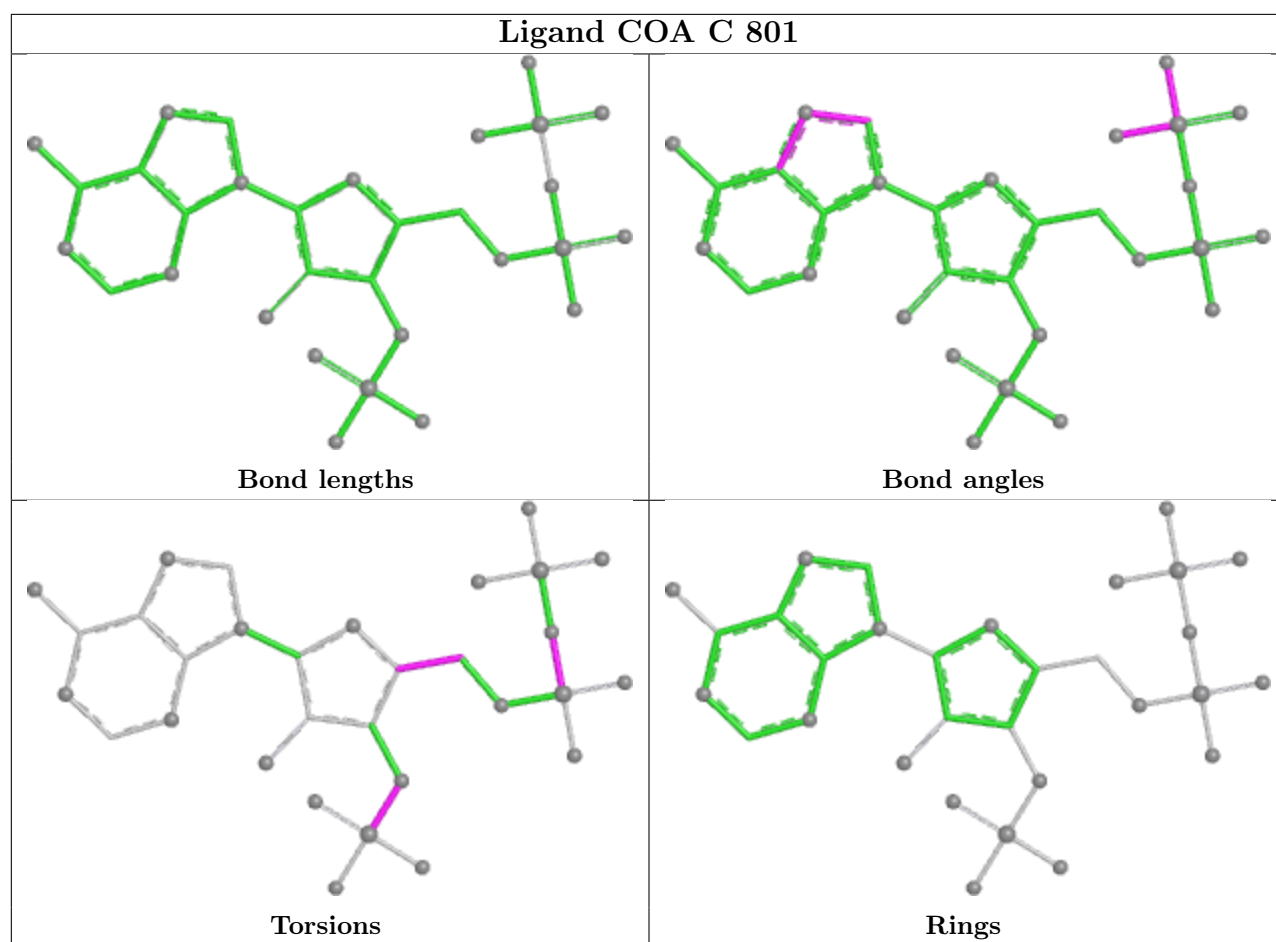
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	COA	1	0
4	A	800	B12	19	0
4	C	800	B12	11	0
3	C	801	COA	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	725/727 (99%)	0.07	17 (2%) 61 57	18, 35, 68, 125	0
1	C	725/727 (99%)	0.04	23 (3%) 50 46	14, 34, 68, 125	0
2	B	619/637 (97%)	0.60	48 (7%) 19 17	19, 51, 99, 129	0
2	D	619/637 (97%)	0.56	38 (6%) 27 23	19, 52, 99, 130	0
All	All	2688/2728 (98%)	0.30	126 (4%) 36 32	14, 42, 87, 130	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	518	LEU	5.0
1	C	476	PRO	4.5
1	A	480	VAL	4.5
1	C	93	SER	4.3
2	B	519	GLY	4.3
1	A	478	LEU	4.2
1	A	92	PHE	4.0
2	B	525	GLY	3.9
2	D	637	ALA	3.8
2	D	545	VAL	3.8
2	D	524	PHE	3.6
1	C	92	PHE	3.5
1	A	483	VAL	3.3
2	D	546	GLU	3.3
1	C	108	ALA	3.2
2	D	602	PHE	3.2
1	C	484	ASP	3.2
1	C	478	LEU	3.1
1	C	160	GLN	3.1
2	B	634	LEU	3.1
1	A	93	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	474	HIS	3.0
2	D	553	ILE	3.0
2	D	573	VAL	3.0
2	D	518	LEU	3.0
2	D	517	CYS	3.0
2	D	523	ASP	3.0
1	C	483	VAL	3.0
1	A	477	PRO	3.0
2	B	159	LEU	3.0
1	C	479	ASP	3.0
2	B	204	PHE	3.0
2	D	217	LEU	2.9
2	B	633	ILE	2.9
2	B	574	TYR	2.9
2	D	606	ALA	2.8
2	D	600	LYS	2.8
1	A	481	LEU	2.8
1	C	110	GLN	2.8
2	D	550	THR	2.8
1	C	475	GLU	2.8
2	B	602	PHE	2.8
2	D	561	GLY	2.7
1	C	107	ALA	2.7
2	B	571	ALA	2.7
2	D	609	ALA	2.7
1	A	475	GLU	2.7
2	D	557	PHE	2.7
2	B	588	ALA	2.7
1	C	140	GLY	2.7
2	B	631	LEU	2.7
2	B	553	ILE	2.6
2	B	573	VAL	2.6
2	D	613	ILE	2.6
1	C	94	THR	2.6
2	B	637	ALA	2.6
2	B	607	ALA	2.6
2	B	577	GLN	2.5
2	D	577	GLN	2.5
2	B	550	THR	2.5
2	D	564	VAL	2.5
2	B	628	SER	2.5
2	D	549	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	138	MET	2.5
1	A	109	GLY	2.5
2	B	520	THR	2.5
2	D	520	THR	2.5
1	C	97	GLU	2.4
2	B	555	GLU	2.4
1	C	89	TYR	2.4
2	D	522	ARG	2.4
1	A	108	ALA	2.4
2	B	150	LEU	2.4
1	C	480	VAL	2.4
2	D	507	VAL	2.4
2	B	606	ALA	2.4
2	B	546	GLU	2.4
2	B	572	LYS	2.4
2	B	523	ASP	2.3
1	A	482	LYS	2.3
2	B	557	PHE	2.3
2	D	263	VAL	2.3
2	D	433	VAL	2.3
2	B	180	VAL	2.3
1	C	485	ASN	2.3
2	D	603	GLY	2.3
1	A	152	LEU	2.3
2	B	524	PHE	2.3
2	B	216	VAL	2.3
2	B	423	VAL	2.3
2	B	603	GLY	2.2
1	C	481	LEU	2.2
2	D	627	LEU	2.2
2	B	554	VAL	2.2
2	D	49	PRO	2.2
2	B	598	ALA	2.2
2	D	598	ALA	2.2
1	A	111	LYS	2.2
2	B	187	ASP	2.2
2	B	516	ALA	2.2
2	D	519	GLY	2.2
2	B	521	ARG	2.2
1	C	106	LEU	2.2
1	A	137	GLY	2.1
2	D	525	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	568	CYS	2.1
1	C	127	SER	2.1
2	B	185	ARG	2.1
2	B	532	SER	2.1
2	B	575	ALA	2.1
1	A	484	ASP	2.1
2	B	569	SER	2.1
2	B	513	VAL	2.1
2	B	214	LEU	2.1
2	B	183	TYR	2.1
2	B	605	ASP	2.1
2	D	566	ASP	2.1
2	D	570	SER	2.1
2	B	522	ARG	2.1
2	D	571	ALA	2.0
2	D	634	LEU	2.0
2	D	578	GLY	2.0
2	D	608	GLU	2.0
1	A	8	ASP	2.0
2	B	153	VAL	2.0
1	C	576	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

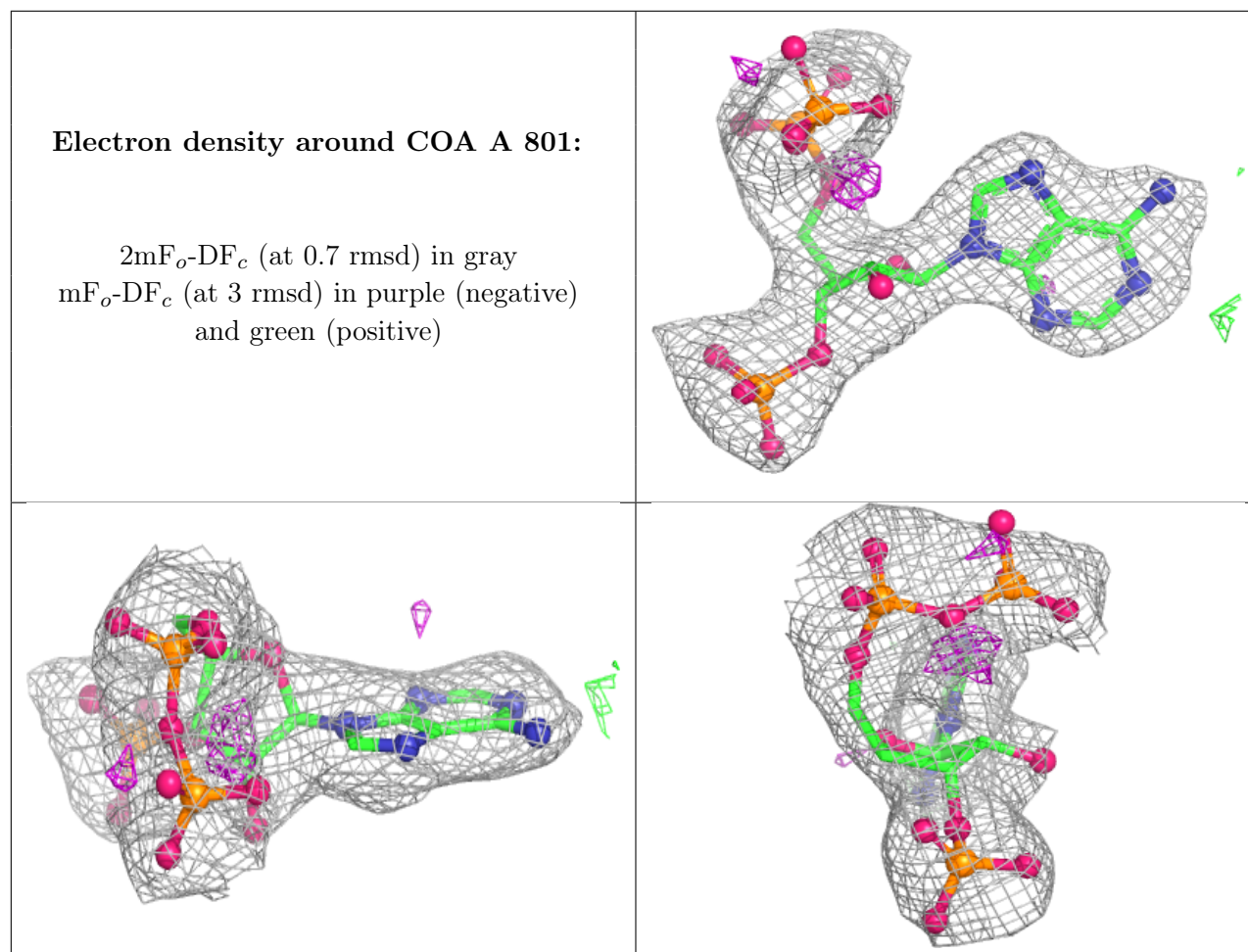
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	COA	A	801	31/48	0.80	0.10	48,79,100,101	0
3	COA	C	801	31/48	0.82	0.11	43,77,100,101	0

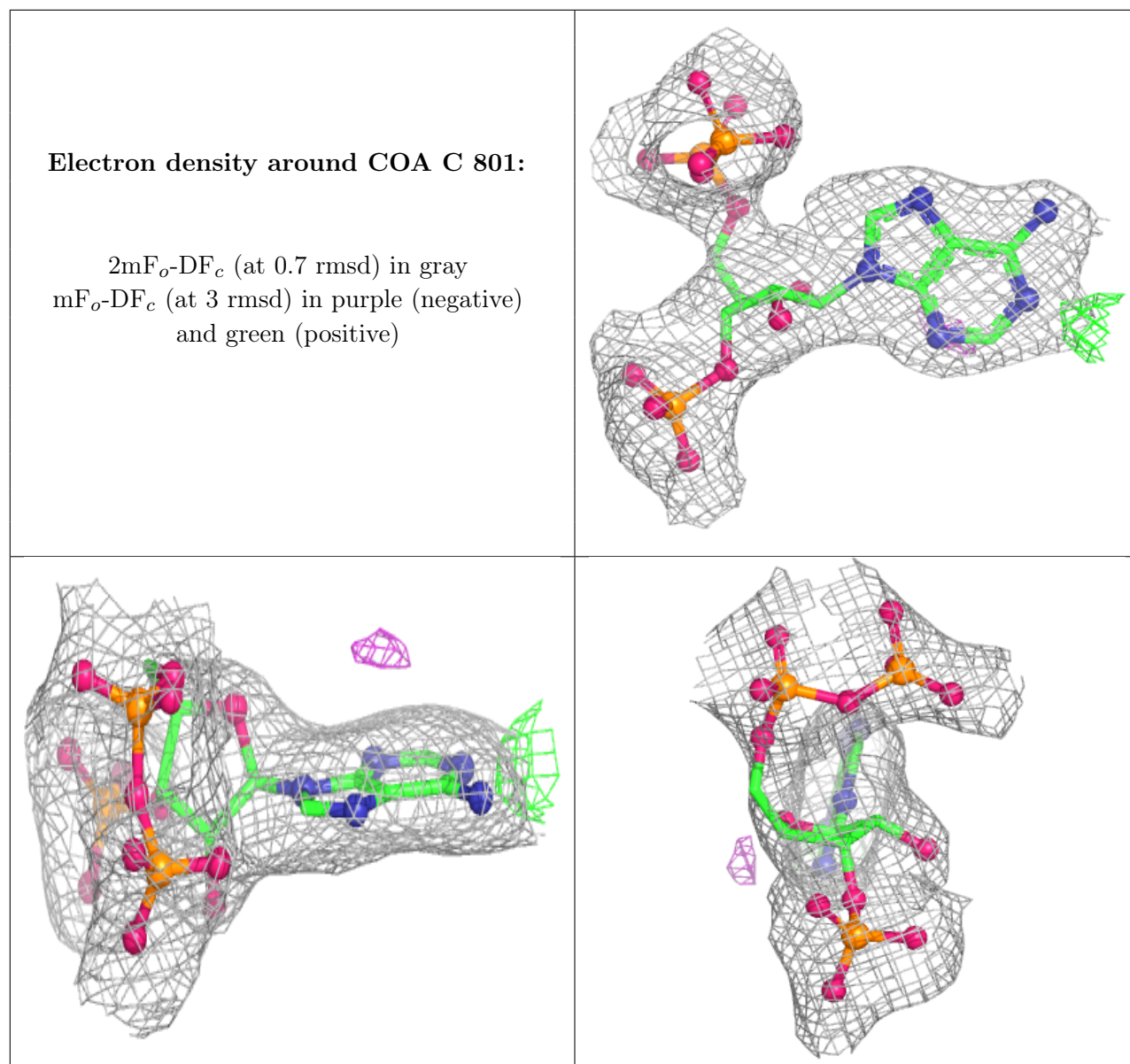
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	B12	A	800	91/91	0.96	0.08	14,27,39,45	0
4	B12	C	800	91/91	0.98	0.07	9,22,33,41	0

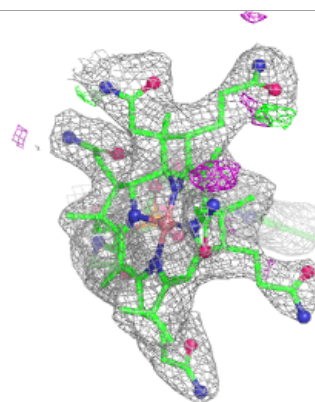
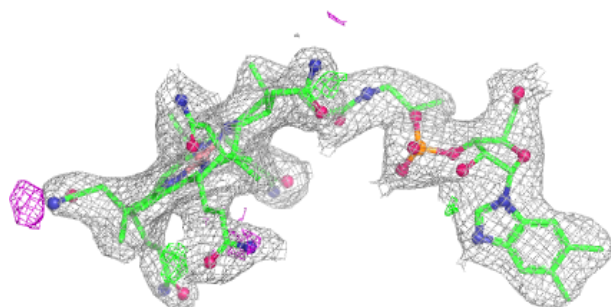
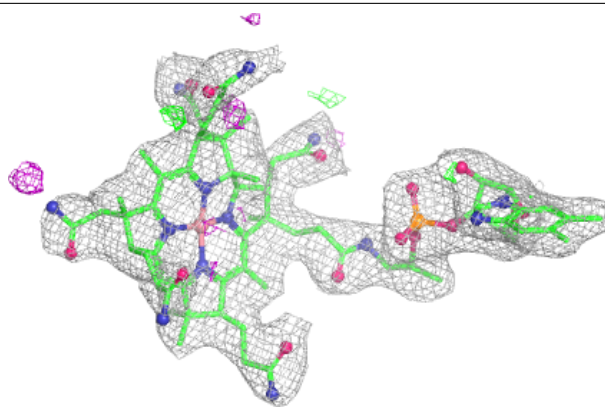
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



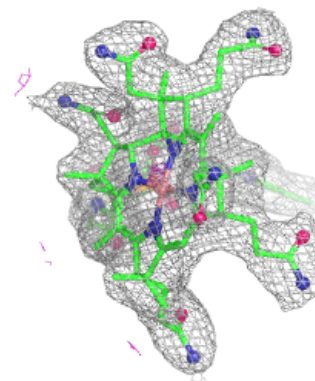
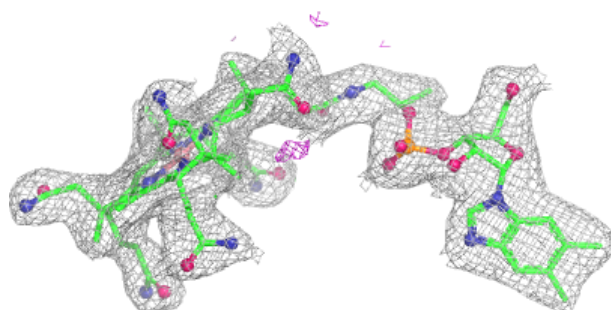
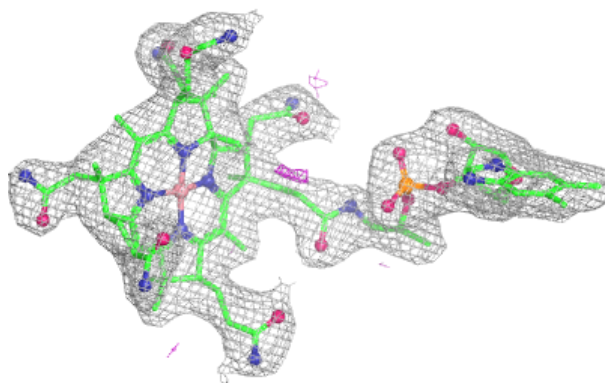


Electron density around B12 A 800:

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

**Electron density around B12 C 800:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.