



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:38 AM UTC

PDB ID : 4REQ / pdb_00004req
Title : Methylmalonyl-CoA Mutase substrate complex
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1998-06-17
Resolution : 2.20 Å(reported)

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

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

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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

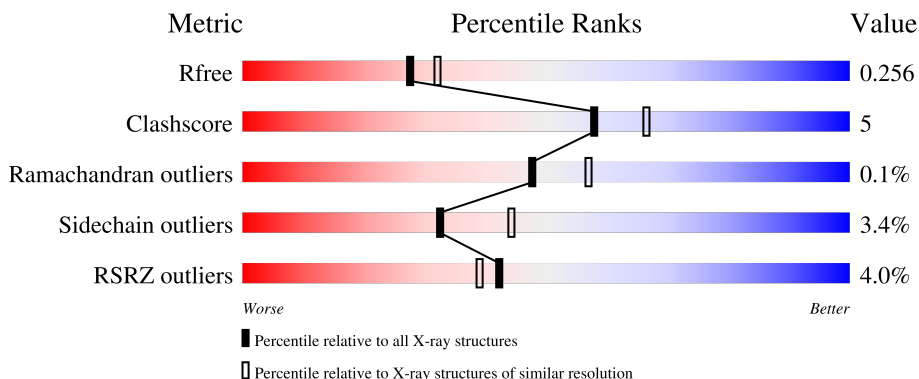
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	727	
1	C	727	
2	B	637	
2	D	637	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22334 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	726	5575	3526	966	1059	24	0	0	0
1	C	726	5575	3526	966	1059	24	0	0	0

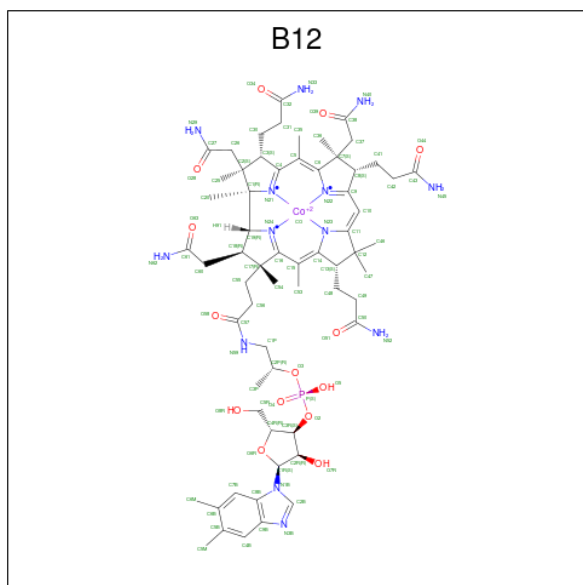
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	4718	2977	826	902	13	0	0	0
2	D	619	4718	2977	826	902	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

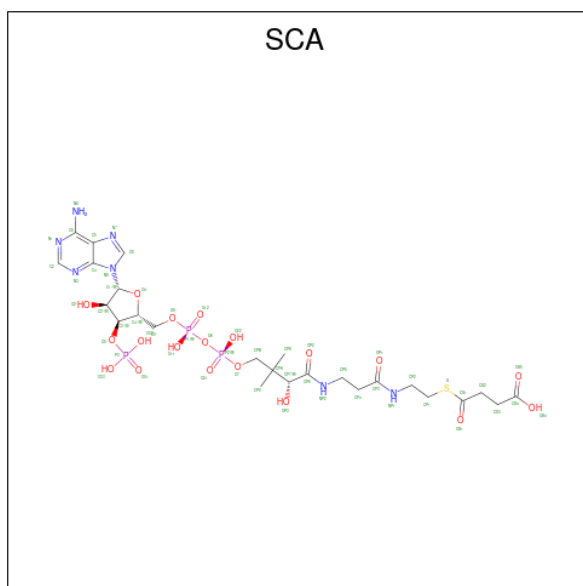
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

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



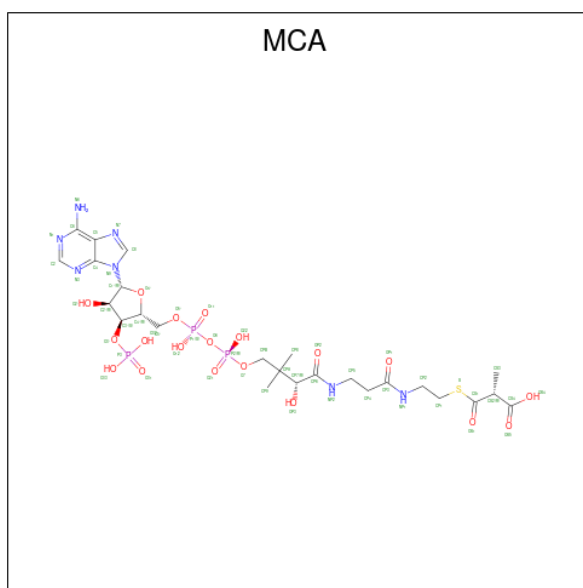
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
3	A	1	91	62	1	13	14	1	0	0
3	C	1	91	62	1	13	14	1	0	0

- Molecule 4 is SUCCINYL-COENZYME A (CCD ID: SCA) (formula: $C_{25}H_{40}N_7O_{19}P_3S$).



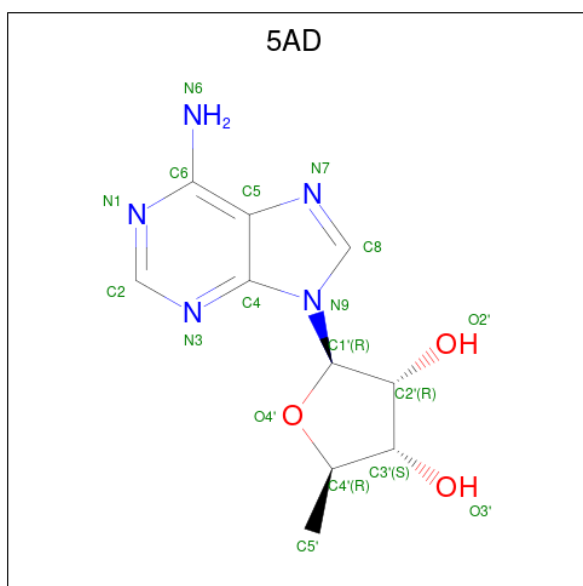
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	55	25	7	19	3	1	0	1
4	C	1	55	25	7	19	3	1	0	1

- Molecule 5 is METHYLMALONYL-COENZYME A (CCD ID: MCA) (formula: $C_{25}H_{40}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	A	1	55	25	7	19	3	1	0	1
5	C	1	55	25	7	19	3	1	0	1

- Molecule 6 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	18	10	5	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	18	10	5	3	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

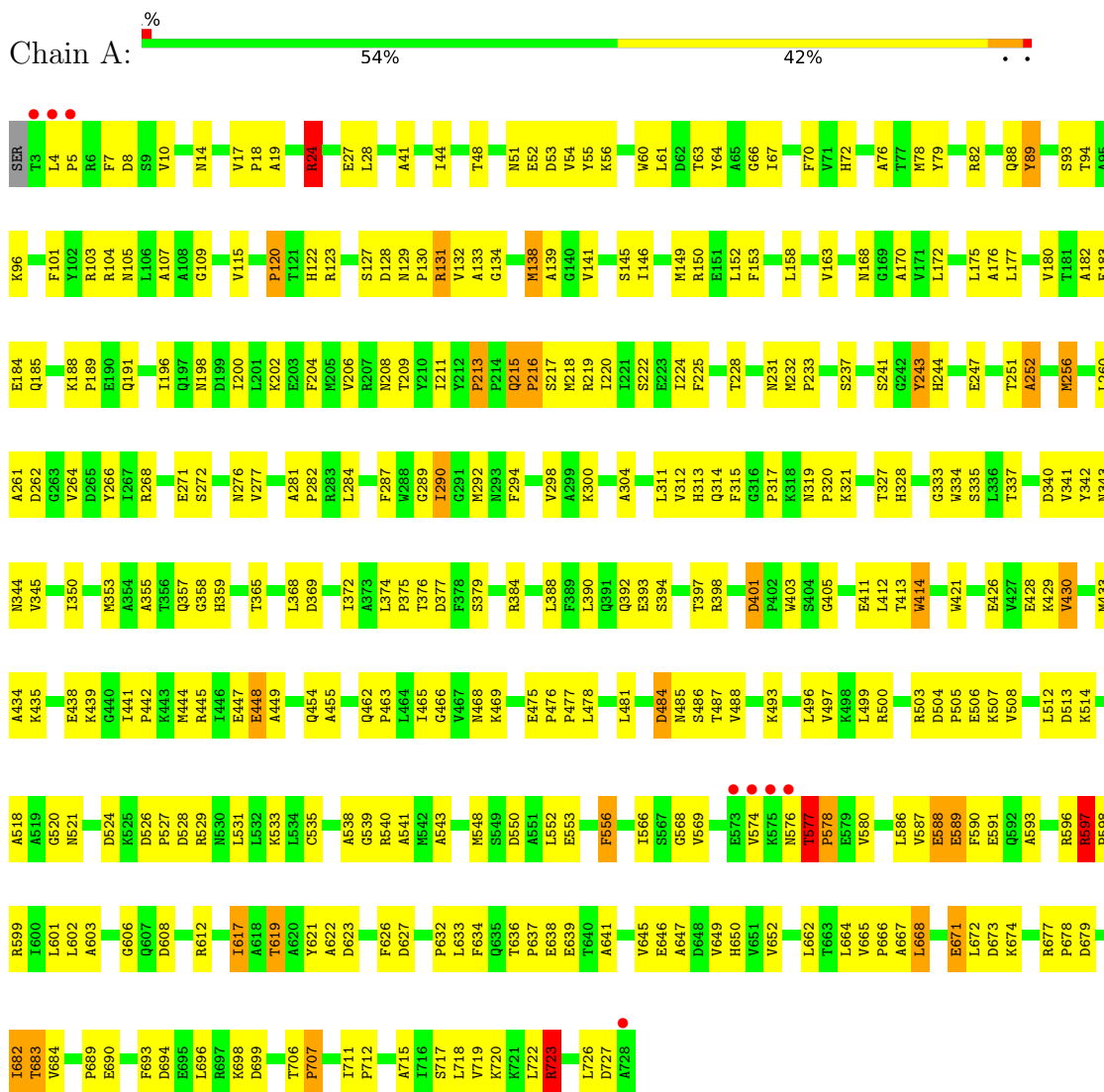
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	404	404	404	0	0
8	B	239	239	239	0	0
8	C	400	400	400	0	0
8	D	243	243	243	0	0

3 Residue-property plots [i](#)

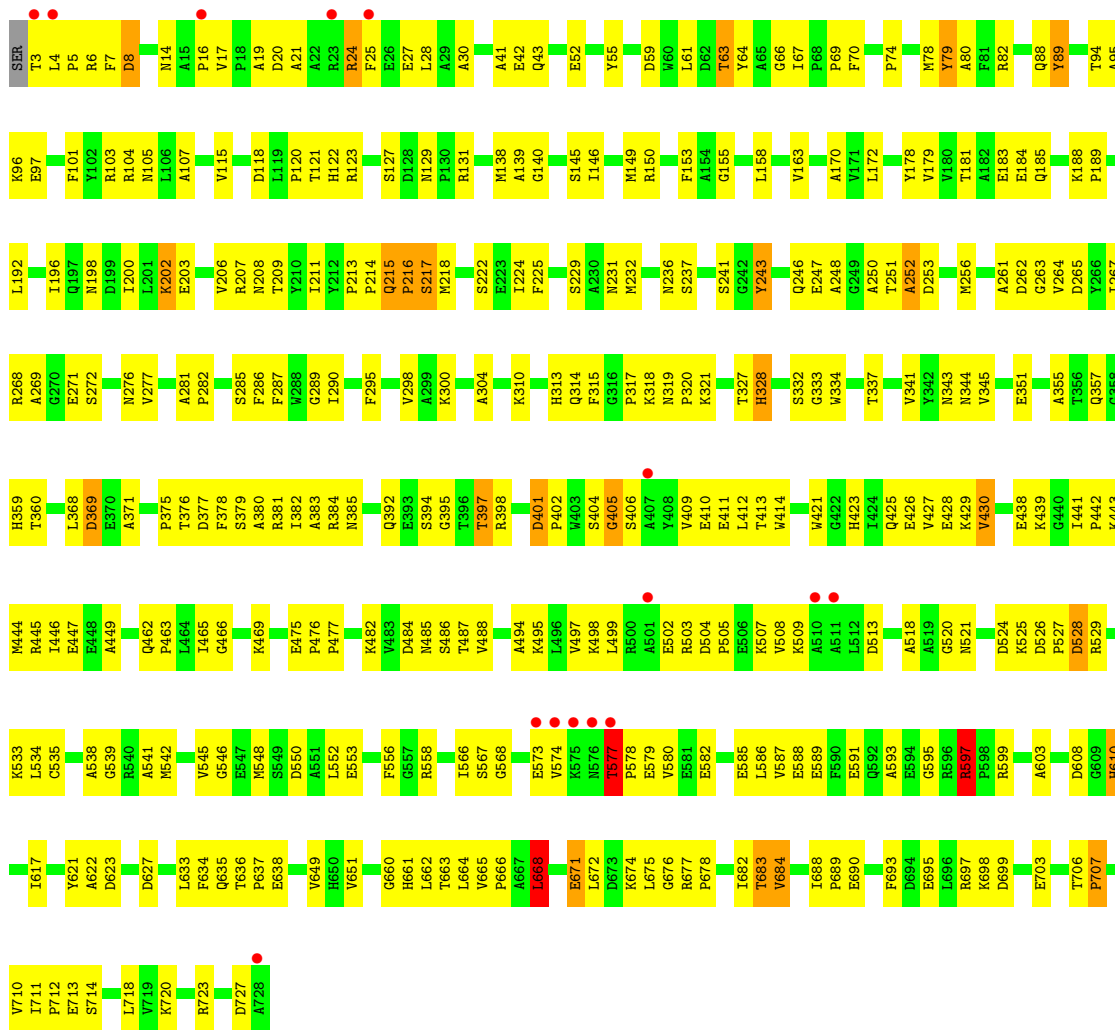
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

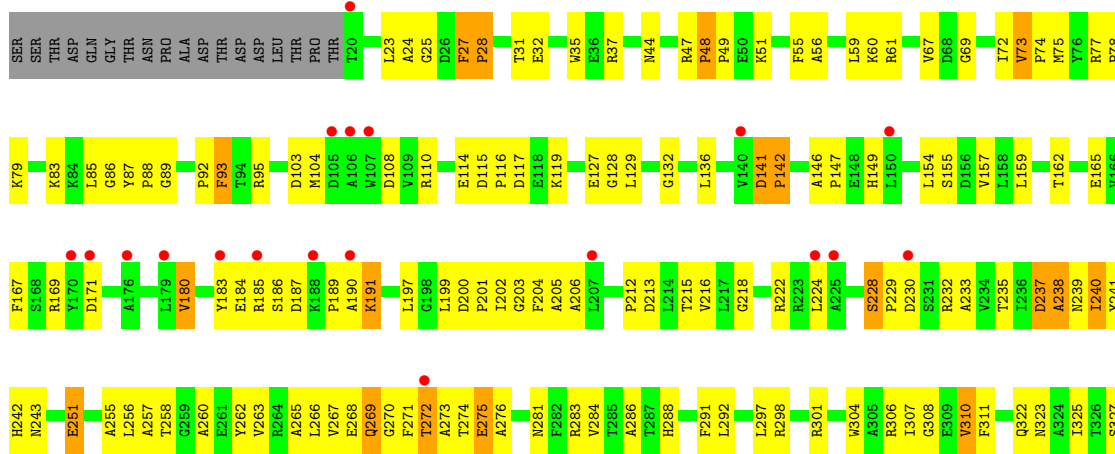


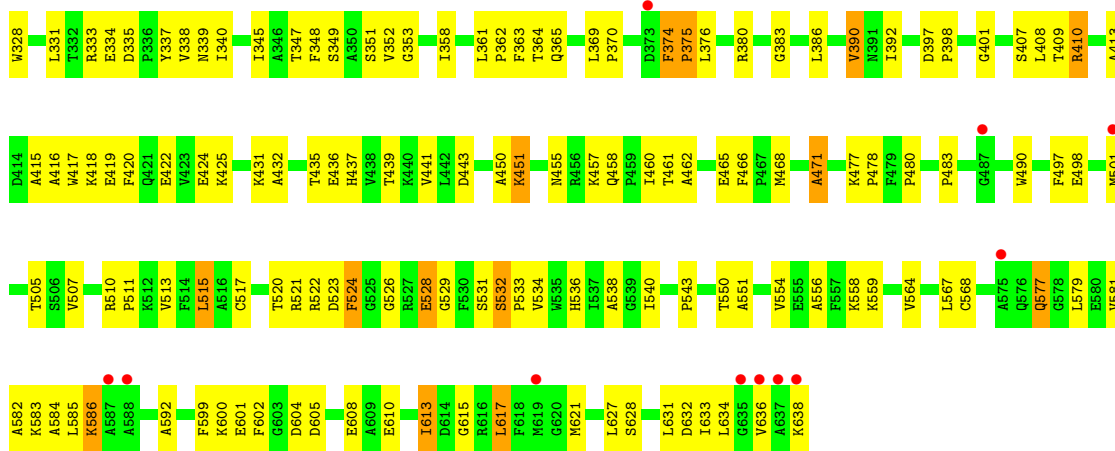
- Molecule 1: METHYLMALONYL-COA MUTASE



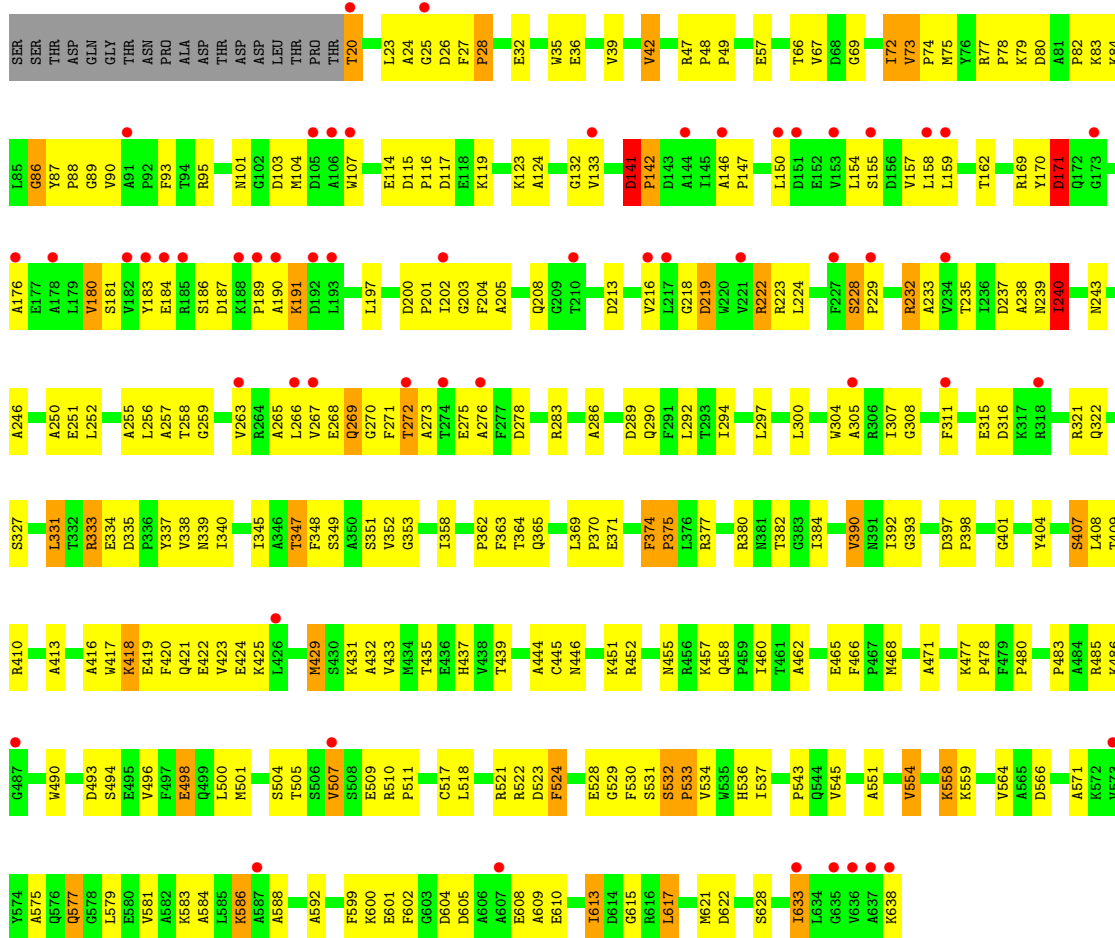


● Molecule 2: METHYLMALONYL-COA MUTASE





● Molecule 2: METHYLMALONYL-COA MUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.13Å 160.90Å 88.50Å 90.00° 104.64° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.8 (20.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.19Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.277 0.214 , 0.256	Depositor DCC
R_{free} test set	16334 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22334	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: SCA, MCA, 5AD, GOL, B12

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.88	0/5692	2.67	550/7730 (7.1%)
1	C	0.90	2/5692 (0.0%)	2.60	511/7730 (6.6%)
2	B	0.78	1/4808 (0.0%)	2.53	441/6521 (6.8%)
2	D	0.76	1/4808 (0.0%)	2.56	417/6521 (6.4%)
All	All	0.84	4/21000 (0.0%)	2.59	1919/28502 (6.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	GLU	N-CA	-5.21	1.39	1.46
2	D	530	PHE	N-CA	-5.07	1.40	1.46
2	B	458	GLN	N-CA	-5.04	1.40	1.46
1	C	172	LEU	CA-C	-5.00	1.47	1.52

All (1919) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	ARG	CD-NE-CZ	20.52	153.12	124.40
1	A	384	ARG	CD-NE-CZ	18.99	150.99	124.40
2	D	269	GLN	CA-C-N	15.53	146.88	122.20
2	D	269	GLN	C-N-CA	15.53	146.88	122.20
2	B	457	LYS	CA-C-N	15.50	142.22	123.16
2	B	457	LYS	C-N-CA	15.50	142.22	123.16
2	D	24	ALA	CA-C-N	15.45	137.33	120.03
2	D	24	ALA	C-N-CA	15.45	137.33	120.03
1	A	678	PRO	CA-C-N	14.33	145.09	120.58
1	A	678	PRO	C-N-CA	14.33	145.09	120.58
1	C	41	ALA	CA-C-N	14.00	145.65	121.14
1	C	41	ALA	C-N-CA	14.00	145.65	121.14
1	A	637	PRO	CA-C-N	13.49	138.78	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	637	PRO	C-N-CA	13.49	138.78	120.44
2	D	457	LYS	CA-C-N	13.39	139.64	123.16
2	D	457	LYS	C-N-CA	13.39	139.64	123.16
1	C	241	SER	N-CA-C	12.23	129.40	109.95
1	A	241	SER	N-CA-C	12.04	129.51	109.76
1	C	597	ARG	CD-NE-CZ	12.03	141.25	124.40
1	C	690	GLU	CA-C-N	11.98	137.88	120.38
1	C	690	GLU	C-N-CA	11.98	137.88	120.38
1	A	597	ARG	CD-NE-CZ	11.77	140.87	124.40
2	D	339	ASN	CA-C-N	11.69	135.28	120.56
2	D	339	ASN	C-N-CA	11.69	135.28	120.56
2	D	132	GLY	N-CA-C	11.56	130.24	115.21
1	A	41	ALA	CA-C-N	11.26	139.52	120.72
1	A	41	ALA	C-N-CA	11.26	139.52	120.72
2	D	239	ASN	CA-C-N	11.25	134.74	120.56
2	D	239	ASN	C-N-CA	11.25	134.74	120.56
2	D	601	GLU	CA-C-N	11.23	142.95	122.06
2	D	601	GLU	C-N-CA	11.23	142.95	122.06
1	A	146	ILE	CA-C-N	11.09	134.86	120.44
1	A	146	ILE	C-N-CA	11.09	134.86	120.44
1	A	369	ASP	CA-C-N	11.07	135.54	120.38
1	A	369	ASP	C-N-CA	11.07	135.54	120.38
1	C	637	PRO	CA-C-N	11.06	135.48	120.44
1	C	637	PRO	C-N-CA	11.06	135.48	120.44
2	B	339	ASN	CA-C-N	11.05	134.49	120.56
2	B	339	ASN	C-N-CA	11.05	134.49	120.56
1	A	690	GLU	CA-C-N	10.92	138.07	120.60
1	A	690	GLU	C-N-CA	10.92	138.07	120.60
2	B	269	GLN	CA-C-N	10.62	141.27	122.05
2	B	269	GLN	C-N-CA	10.62	141.27	122.05
1	C	41	ALA	O-C-N	-10.59	110.12	122.20
1	C	146	ILE	CA-C-N	10.51	134.72	120.54
1	C	146	ILE	C-N-CA	10.51	134.72	120.54
2	B	601	GLU	CA-C-N	10.45	141.96	121.58
2	B	601	GLU	C-N-CA	10.45	141.96	121.58
1	C	476	PRO	N-CA-CB	10.41	109.02	103.19
1	A	262	ASP	CA-C-N	10.36	131.47	119.98
1	A	262	ASP	C-N-CA	10.36	131.47	119.98
2	D	89	GLY	CA-C-N	10.30	137.54	122.71
2	D	89	GLY	C-N-CA	10.30	137.54	122.71
2	D	238	ALA	CA-C-N	10.29	137.91	120.72
2	D	238	ALA	C-N-CA	10.29	137.91	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	307	ILE	CA-C-N	10.25	131.58	119.99
2	D	307	ILE	C-N-CA	10.25	131.58	119.99
2	B	239	ASN	CA-C-N	10.24	134.18	120.77
2	B	239	ASN	C-N-CA	10.24	134.18	120.77
2	B	437	HIS	CA-CB-CG	-10.21	103.59	113.80
2	D	528	GLU	CA-C-N	10.14	131.39	120.03
2	D	528	GLU	C-N-CA	10.14	131.39	120.03
1	C	690	GLU	O-C-N	-10.13	111.38	122.12
2	B	86	GLY	O-C-N	-10.10	111.07	122.68
1	A	131	ARG	CD-NE-CZ	10.01	138.41	124.40
2	B	89	GLY	CA-C-N	10.00	137.10	122.71
2	B	89	GLY	C-N-CA	10.00	137.10	122.71
2	B	613	ILE	CA-C-O	9.93	131.93	120.71
1	C	327	THR	N-CA-C	9.92	125.17	109.50
1	C	369	ASP	CA-C-N	9.89	135.66	120.82
1	C	369	ASP	C-N-CA	9.89	135.66	120.82
2	D	352	VAL	CA-C-N	9.87	138.36	120.79
2	D	352	VAL	C-N-CA	9.87	138.36	120.79
1	A	8	ASP	CA-C-N	9.78	137.82	122.26
1	A	8	ASP	C-N-CA	9.78	137.82	122.26
2	B	32	GLU	CA-C-N	9.79	133.75	120.54
2	B	32	GLU	C-N-CA	9.79	133.75	120.54
1	A	693	PHE	CA-CB-CG	9.72	123.52	113.80
1	A	327	THR	N-CA-C	9.72	124.58	109.52
2	B	103	ASP	CA-CB-CG	-9.61	102.99	112.60
1	A	497	VAL	N-CA-C	-9.61	101.50	110.53
1	A	70	PHE	CA-CB-CG	9.59	123.39	113.80
2	B	450	ALA	CA-C-N	9.59	132.91	120.44
2	B	450	ALA	C-N-CA	9.59	132.91	120.44
2	D	337	TYR	CA-C-N	9.57	135.59	120.47
2	D	337	TYR	C-N-CA	9.57	135.59	120.47
2	B	238	ALA	CA-C-N	9.54	134.02	120.28
2	B	238	ALA	C-N-CA	9.54	134.02	120.28
2	B	339	ASN	O-C-N	-9.51	110.03	122.39
2	B	263	VAL	N-CA-C	-9.43	101.66	110.53
1	A	476	PRO	N-CA-CB	9.42	108.46	103.19
1	A	215	GLN	CA-C-O	9.42	128.03	119.08
2	D	72	ILE	CB-CG1-CD1	9.41	133.56	113.80
1	A	334	TRP	O-C-N	-9.37	112.18	122.12
1	C	333	GLY	CA-C-N	9.34	132.80	120.28
1	C	333	GLY	C-N-CA	9.34	132.80	120.28
1	C	63	THR	CA-C-N	9.30	136.41	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	THR	C-N-CA	9.30	136.41	122.93
2	D	169	ARG	CD-NE-CZ	9.27	137.38	124.40
1	C	343	ASN	CA-C-N	9.21	133.55	120.28
1	C	343	ASN	C-N-CA	9.21	133.55	120.28
2	D	243	ASN	CA-C-N	9.18	139.13	122.06
2	D	243	ASN	C-N-CA	9.18	139.13	122.06
2	D	263	VAL	N-CA-C	-9.16	101.81	110.42
1	C	321	LYS	O-C-N	-9.15	111.51	122.22
1	A	333	GLY	O-C-N	-9.10	113.37	122.19
1	A	429	LYS	CA-C-N	9.07	135.59	121.34
1	A	429	LYS	C-N-CA	9.07	135.59	121.34
1	C	333	GLY	O-C-N	-9.05	113.41	122.19
1	A	261	ALA	O-C-N	-9.03	111.85	122.15
2	D	203	GLY	CA-C-N	9.00	132.14	120.44
2	D	203	GLY	C-N-CA	9.00	132.14	120.44
2	B	77	ARG	CD-NE-CZ	9.00	137.00	124.40
2	D	601	GLU	O-C-N	-8.99	110.47	122.43
1	A	185	GLN	CA-C-N	8.98	135.46	120.91
1	A	185	GLN	C-N-CA	8.98	135.46	120.91
2	B	117	ASP	CA-CB-CG	8.98	121.58	112.60
1	C	410	GLU	CA-C-O	-8.97	110.91	120.42
1	A	679	ASP	CA-CB-CG	8.96	121.56	112.60
2	D	435	THR	CA-CB-CG2	8.96	125.73	110.50
1	A	633	LEU	O-C-N	-8.95	111.73	122.65
2	B	528	GLU	CA-C-N	8.93	131.31	120.14
2	B	528	GLU	C-N-CA	8.93	131.31	120.14
2	D	339	ASN	O-C-N	-8.92	111.78	122.22
1	A	342	TYR	CA-C-N	8.91	133.85	120.31
1	A	342	TYR	C-N-CA	8.91	133.85	120.31
2	D	269	GLN	O-C-N	-8.90	110.75	122.59
1	A	398	ARG	N-CA-C	8.87	121.91	111.71
1	C	8	ASP	CA-C-N	8.87	136.17	122.24
1	C	8	ASP	C-N-CA	8.87	136.17	122.24
1	A	633	LEU	CA-C-N	8.86	135.10	122.08
1	A	633	LEU	C-N-CA	8.86	135.10	122.08
1	C	24	ARG	CD-NE-CZ	8.84	136.78	124.40
1	A	439	LYS	CA-C-N	8.82	138.91	121.53
1	A	439	LYS	C-N-CA	8.82	138.91	121.53
1	A	231	ASN	OD1-CG-ND2	8.80	131.40	122.60
1	A	556	PHE	N-CA-C	8.80	123.32	112.23
2	B	536	HIS	O-C-N	-8.78	110.97	122.39
1	C	52	GLU	O-C-N	-8.78	110.75	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	633	LEU	O-C-N	-8.77	111.95	122.65
1	A	228	THR	O-C-N	-8.76	113.05	122.07
1	A	723	ARG	CD-NE-CZ	8.76	136.66	124.40
1	C	633	LEU	CA-C-O	8.76	131.97	121.99
1	C	462	GLN	CA-C-O	8.75	126.71	119.36
2	D	377	ARG	CD-NE-CZ	8.74	136.64	124.40
2	D	353	GLY	CA-C-N	8.71	135.80	121.00
2	D	353	GLY	C-N-CA	8.71	135.80	121.00
1	C	78	MET	CA-C-N	8.70	135.26	120.72
1	C	78	MET	C-N-CA	8.70	135.26	120.72
1	A	52	GLU	O-C-N	-8.70	111.08	122.39
2	B	435	THR	CA-CB-CG2	8.70	125.29	110.50
2	D	409	THR	N-CA-C	-8.70	101.75	111.14
2	B	72	ILE	CB-CG1-CD1	8.69	132.04	113.80
2	D	24	ALA	O-C-N	-8.69	111.58	122.27
2	D	255	ALA	N-CA-C	-8.68	100.81	111.40
1	C	665	VAL	CA-C-O	8.65	124.48	118.69
1	C	281	ALA	O-C-N	-8.65	112.78	120.48
1	A	333	GLY	CA-C-N	8.63	131.85	120.28
1	A	333	GLY	C-N-CA	8.63	131.85	120.28
1	C	183	GLU	O-C-N	-8.62	113.12	122.09
1	A	215	GLN	O-C-N	-8.61	113.58	120.38
1	C	52	GLU	CA-C-N	8.61	135.10	120.72
1	C	52	GLU	C-N-CA	8.61	135.10	120.72
1	A	287	PHE	CA-CB-CG	8.61	122.41	113.80
2	B	132	GLY	N-CA-C	8.61	126.40	115.21
1	C	608	ASP	CA-CB-CG	8.58	121.18	112.60
1	A	282	PRO	O-C-N	-8.58	110.74	122.24
1	A	673	ASP	O-C-N	-8.56	113.12	122.03
2	D	78	PRO	CA-C-N	8.55	134.28	120.60
2	D	78	PRO	C-N-CA	8.55	134.28	120.60
1	A	272	SER	CA-C-N	8.54	134.41	122.28
1	A	272	SER	C-N-CA	8.54	134.41	122.28
2	D	268	GLU	N-CA-C	-8.54	101.67	110.97
1	A	343	ASN	CA-C-N	8.53	132.57	120.28
1	A	343	ASN	C-N-CA	8.53	132.57	120.28
2	B	25	GLY	O-C-N	-8.52	113.17	122.54
1	A	641	ALA	CA-C-N	8.52	131.51	120.44
1	A	641	ALA	C-N-CA	8.52	131.51	120.44
1	A	535	CYS	CA-C-N	8.51	131.29	120.56
1	A	535	CYS	C-N-CA	8.51	131.29	120.56
1	A	412	LEU	CA-C-N	8.49	131.48	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	LEU	C-N-CA	8.49	131.48	120.44
1	A	224	ILE	N-CA-C	-8.49	102.15	110.72
2	B	600	LYS	CA-C-N	8.48	134.88	120.72
2	B	600	LYS	C-N-CA	8.48	134.88	120.72
2	D	600	LYS	O-C-N	-8.47	111.85	122.27
1	C	664	LEU	CA-C-N	8.46	127.10	120.33
1	C	664	LEU	C-N-CA	8.46	127.10	120.33
2	D	600	LYS	CA-C-N	8.46	136.72	120.99
2	D	600	LYS	C-N-CA	8.46	136.72	120.99
1	C	528	ASP	CA-C-N	8.44	136.85	122.26
1	C	528	ASP	C-N-CA	8.44	136.85	122.26
1	C	216	PRO	CA-C-N	8.43	131.40	120.44
1	C	216	PRO	C-N-CA	8.43	131.40	120.44
2	B	243	ASN	CA-C-N	8.43	138.01	121.58
2	B	243	ASN	C-N-CA	8.43	138.01	121.58
2	B	363	PHE	CA-C-N	8.43	138.79	121.94
2	B	363	PHE	C-N-CA	8.43	138.79	121.94
1	C	198	ASN	N-CA-CB	-8.40	99.61	111.62
1	A	712	PRO	CA-C-N	8.39	131.53	120.28
1	A	712	PRO	C-N-CA	8.39	131.53	120.28
1	A	413	THR	CA-C-N	8.39	131.52	120.28
1	A	413	THR	C-N-CA	8.39	131.52	120.28
2	B	340	ILE	CA-C-N	8.39	131.85	120.44
2	B	340	ILE	C-N-CA	8.39	131.85	120.44
2	D	147	PRO	CA-C-N	8.37	135.79	121.14
2	D	147	PRO	C-N-CA	8.37	135.79	121.14
1	A	184	GLU	O-C-N	-8.37	112.66	122.20
1	C	79	TYR	CA-C-N	8.31	131.41	120.28
1	C	79	TYR	C-N-CA	8.31	131.41	120.28
1	A	674	LYS	CA-C-N	8.28	138.50	121.94
1	A	674	LYS	C-N-CA	8.28	138.50	121.94
2	D	78	PRO	O-C-N	-8.28	112.72	122.24
1	C	394	SER	N-CA-C	8.25	121.20	111.71
1	A	216	PRO	CA-C-N	8.25	131.16	120.44
1	A	216	PRO	C-N-CA	8.25	131.16	120.44
2	B	86	GLY	CA-C-O	8.25	130.16	122.57
2	B	628	SER	CA-C-N	8.25	131.16	120.44
2	B	628	SER	C-N-CA	8.25	131.16	120.44
2	B	78	PRO	O-C-N	-8.24	112.76	122.24
2	B	78	PRO	CA-C-N	8.21	133.74	120.60
2	B	78	PRO	C-N-CA	8.21	133.74	120.60
2	D	159	LEU	N-CA-C	8.20	122.55	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	PRO	CA-C-N	8.18	131.24	120.28
1	A	120	PRO	C-N-CA	8.18	131.24	120.28
1	C	202	LYS	CA-C-N	8.18	131.07	120.44
1	C	202	LYS	C-N-CA	8.18	131.07	120.44
1	A	243	TYR	CA-C-N	8.16	131.22	120.28
1	A	243	TYR	C-N-CA	8.16	131.22	120.28
1	A	677	ARG	CA-CB-CG	8.16	130.43	114.10
2	D	229	PRO	CA-C-N	8.15	136.01	121.66
2	D	229	PRO	C-N-CA	8.15	136.01	121.66
2	D	243	ASN	O-C-N	-8.15	111.79	122.39
1	C	282	PRO	CA-C-N	8.15	135.69	122.65
1	C	282	PRO	C-N-CA	8.15	135.69	122.65
1	C	224	ILE	N-CA-C	-8.12	102.14	111.00
2	D	477	LYS	N-CA-C	-8.12	99.56	109.72
2	B	202	ILE	CA-C-N	8.11	129.15	119.99
2	B	202	ILE	C-N-CA	8.11	129.15	119.99
2	B	24	ALA	CA-C-N	8.10	134.66	120.74
2	B	24	ALA	C-N-CA	8.10	134.66	120.74
1	C	447	GLU	O-C-N	-8.08	113.55	122.12
1	A	261	ALA	N-CA-C	-8.07	102.56	111.36
1	A	674	LYS	O-C-N	-8.07	113.00	122.20
2	B	229	PRO	CA-C-N	8.05	135.23	121.14
2	B	229	PRO	C-N-CA	8.05	135.23	121.14
1	C	678	PRO	CA-C-N	8.04	135.20	121.14
1	C	678	PRO	C-N-CA	8.04	135.20	121.14
1	A	319	ASN	CA-C-N	7.98	128.06	119.28
1	A	319	ASN	C-N-CA	7.98	128.06	119.28
2	B	307	ILE	CA-C-N	7.98	129.00	119.99
2	B	307	ILE	C-N-CA	7.98	129.00	119.99
1	A	24	ARG	CD-NE-CZ	7.97	135.56	124.40
1	C	337	THR	CA-C-O	7.97	131.20	121.56
1	A	63	THR	O-C-N	-7.96	111.90	122.97
2	B	601	GLU	O-C-N	-7.96	111.77	122.43
1	A	237	SER	N-CA-C	7.95	122.80	113.18
2	D	141	ASP	CA-CB-CG	7.95	120.55	112.60
2	B	269	GLN	O-C-N	-7.94	112.03	122.59
1	A	645	VAL	O-C-N	-7.94	114.00	121.94
2	B	232	ARG	CD-NE-CZ	7.93	135.51	124.40
1	C	343	ASN	O-C-N	-7.93	111.80	122.43
2	B	243	ASN	O-C-N	-7.92	112.95	122.22
2	D	86	GLY	CA-C-O	7.92	129.85	122.57
1	C	341	VAL	N-CA-C	7.91	123.29	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	MET	CA-C-N	7.91	131.52	120.29
1	C	149	MET	C-N-CA	7.91	131.52	120.29
2	D	69	GLY	N-CA-C	7.91	127.08	114.90
2	B	147	PRO	CA-C-N	7.90	134.97	121.14
2	B	147	PRO	C-N-CA	7.90	134.97	121.14
1	A	79	TYR	CA-C-N	7.90	130.86	120.28
1	A	79	TYR	C-N-CA	7.90	130.86	120.28
2	B	511	PRO	N-CA-CB	7.88	110.21	103.35
1	C	488	VAL	CB-CA-C	-7.88	101.70	112.02
1	A	633	LEU	CA-C-O	7.87	130.96	121.99
1	A	66	GLY	O-C-N	-7.85	112.59	122.41
2	D	67	VAL	CA-C-N	7.84	134.91	122.83
2	D	67	VAL	C-N-CA	7.84	134.91	122.83
1	A	462	GLN	CA-C-O	7.83	125.94	119.36
2	B	425	LYS	CA-C-N	7.83	136.86	121.58
2	B	425	LYS	C-N-CA	7.83	136.86	121.58
1	C	153	PHE	CA-CB-CG	-7.83	105.97	113.80
2	D	337	TYR	O-C-N	-7.83	112.21	122.39
1	C	231	ASN	OD1-CG-ND2	7.83	130.43	122.60
1	A	369	ASP	O-C-N	-7.82	112.36	122.37
2	D	213	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	553	GLU	CA-C-N	7.78	130.56	120.44
1	A	553	GLU	C-N-CA	7.78	130.56	120.44
1	A	593	ALA	CA-C-O	-7.78	112.17	120.42
1	A	577	THR	CA-C-N	7.78	127.83	119.28
1	A	577	THR	C-N-CA	7.78	127.83	119.28
2	B	398	PRO	O-C-N	-7.78	112.19	122.22
1	A	445	ARG	CA-C-N	7.77	130.35	120.56
1	A	445	ARG	C-N-CA	7.77	130.35	120.56
2	B	141	ASP	CA-CB-CG	7.76	120.36	112.60
2	B	338	VAL	O-C-N	-7.75	114.04	121.87
1	C	553	GLU	CA-C-N	7.75	131.01	120.54
1	C	553	GLU	C-N-CA	7.75	131.01	120.54
1	A	220	ILE	CA-C-N	7.75	130.33	120.56
1	A	220	ILE	C-N-CA	7.75	130.33	120.56
2	D	422	GLU	CA-C-N	7.75	131.08	120.46
2	D	422	GLU	C-N-CA	7.75	131.08	120.46
1	C	321	LYS	CA-C-N	7.74	131.69	120.38
1	C	321	LYS	C-N-CA	7.74	131.69	120.38
1	C	693	PHE	CA-CB-CG	7.74	121.54	113.80
1	A	664	LEU	N-CA-C	7.73	119.70	111.28
2	D	364	THR	CA-C-N	7.71	131.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	364	THR	C-N-CA	7.71	131.63	120.38
2	D	390	VAL	O-C-N	-7.70	113.09	122.18
1	A	52	GLU	CA-C-N	7.69	132.91	120.60
1	A	52	GLU	C-N-CA	7.69	132.91	120.60
1	A	438	GLU	O-C-N	-7.69	114.09	122.09
2	B	327	SER	N-CA-C	7.69	121.42	109.96
1	C	313	HIS	O-C-N	-7.69	113.97	122.12
1	C	351	GLU	CA-C-N	7.68	130.57	120.28
1	C	351	GLU	C-N-CA	7.68	130.57	120.28
1	A	206	VAL	CB-CA-C	-7.67	98.71	111.29
2	B	536	HIS	CA-C-N	7.67	131.34	120.53
2	B	536	HIS	C-N-CA	7.67	131.34	120.53
1	A	313	HIS	CA-C-N	7.66	132.86	120.60
1	A	313	HIS	C-N-CA	7.66	132.86	120.60
2	D	162	THR	N-CA-C	7.66	121.01	108.52
2	B	586	LYS	CA-C-N	7.66	131.16	120.29
2	B	586	LYS	C-N-CA	7.66	131.16	120.29
2	D	322	GLN	CA-C-O	7.66	128.97	120.70
2	B	154	LEU	CA-C-N	7.64	130.85	120.54
2	B	154	LEU	C-N-CA	7.64	130.85	120.54
1	A	41	ALA	O-C-N	-7.62	113.30	122.22
1	A	603	ALA	N-CA-C	7.62	122.26	109.76
1	A	662	LEU	CA-C-O	-7.62	112.40	120.63
1	C	314	GLN	CA-C-N	7.62	136.24	122.06
1	C	314	GLN	C-N-CA	7.62	136.24	122.06
2	B	353	GLY	CA-C-N	7.61	133.93	121.00
2	B	353	GLY	C-N-CA	7.61	133.93	121.00
2	D	25	GLY	O-C-N	-7.59	114.80	122.17
2	D	117	ASP	CA-CB-CG	7.59	120.19	112.60
1	A	170	ALA	CA-C-N	7.58	130.84	120.46
1	A	170	ALA	C-N-CA	7.58	130.84	120.46
2	D	462	ALA	CA-C-N	7.56	135.58	121.97
2	D	462	ALA	C-N-CA	7.56	135.58	121.97
1	A	394	SER	N-CA-C	7.55	120.39	111.71
1	C	170	ALA	CA-C-N	7.55	130.81	120.46
1	C	170	ALA	C-N-CA	7.55	130.81	120.46
2	D	289	ASP	CA-CB-CG	-7.54	105.06	112.60
2	D	446	ASN	CA-C-O	-7.54	112.56	120.55
1	A	313	HIS	O-C-N	-7.53	114.14	122.12
2	B	397	ASP	CA-C-N	7.53	127.56	119.28
2	B	397	ASP	C-N-CA	7.53	127.56	119.28
1	C	412	LEU	O-C-N	-7.50	114.17	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	146	ALA	CA-C-N	7.50	127.53	119.28
2	D	146	ALA	C-N-CA	7.50	127.53	119.28
1	C	438	GLU	O-C-N	-7.47	114.20	122.12
1	C	209	THR	N-CA-CB	7.47	123.89	111.49
1	C	146	ILE	O-C-N	-7.47	114.57	121.89
1	A	55	TYR	N-CA-C	7.46	120.29	111.71
1	C	261	ALA	O-C-N	-7.46	113.65	122.15
2	D	202	ILE	CA-C-N	7.46	128.41	119.99
2	D	202	ILE	C-N-CA	7.46	128.41	119.99
1	C	546	GLY	CA-C-O	-7.45	112.95	121.00
2	B	633	ILE	O-C-N	-7.45	114.59	121.89
2	D	586	LYS	CA-C-N	7.44	130.25	120.28
2	D	586	LYS	C-N-CA	7.44	130.25	120.28
2	B	256	LEU	CA-C-N	7.44	130.11	120.44
2	B	256	LEU	C-N-CA	7.44	130.11	120.44
1	C	5	PRO	N-CA-CB	7.44	109.82	103.35
1	C	225	PHE	CA-CB-CG	7.43	121.23	113.80
2	B	409	THR	N-CA-C	-7.42	103.14	111.07
1	A	428	GLU	CA-C-N	7.41	130.21	120.28
1	A	428	GLU	C-N-CA	7.41	130.21	120.28
1	C	499	LEU	CA-C-N	7.39	130.18	120.28
1	C	499	LEU	C-N-CA	7.39	130.18	120.28
1	C	524	ASP	CA-CB-CG	7.39	119.99	112.60
2	B	352	VAL	O-C-N	-7.38	113.46	121.80
2	B	424	GLU	CA-C-N	7.38	130.91	120.28
2	B	424	GLU	C-N-CA	7.38	130.91	120.28
2	D	25	GLY	CA-C-N	7.38	135.96	121.58
2	D	25	GLY	C-N-CA	7.38	135.96	121.58
2	B	48	PRO	CA-C-N	7.37	128.02	119.47
2	B	48	PRO	C-N-CA	7.37	128.02	119.47
1	A	340	ASP	CA-C-N	7.36	132.10	120.47
1	A	340	ASP	C-N-CA	7.36	132.10	120.47
1	A	588	GLU	CA-C-N	7.35	130.12	120.28
1	A	588	GLU	C-N-CA	7.35	130.12	120.28
2	D	47	ARG	CA-C-O	7.34	125.68	119.66
1	A	281	ALA	O-C-N	-7.34	113.95	120.48
1	A	574	VAL	N-CA-CB	7.34	120.99	112.40
1	A	639	GLU	CA-C-N	7.34	130.72	120.29
1	A	639	GLU	C-N-CA	7.34	130.72	120.29
1	C	298	VAL	O-C-N	-7.34	114.72	121.91
2	D	437	HIS	CA-CB-CG	-7.32	106.48	113.80
1	C	421	TRP	CA-C-N	7.32	128.06	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	TRP	C-N-CA	7.32	128.06	119.94
1	A	520	GLY	O-C-N	-7.31	113.50	122.71
1	A	637	PRO	O-C-N	-7.30	112.81	122.22
2	D	432	ALA	CA-C-N	7.30	130.78	120.42
2	D	432	ALA	C-N-CA	7.30	130.78	120.42
2	D	86	GLY	O-C-N	-7.28	114.30	122.68
2	B	159	LEU	N-CA-C	7.28	121.26	112.38
1	A	268	ARG	NE-CZ-NH2	-7.27	112.65	119.20
2	B	375	PRO	CA-C-N	7.27	129.89	120.44
2	B	375	PRO	C-N-CA	7.27	129.89	120.44
2	D	466	PHE	O-C-N	-7.27	118.19	121.53
1	C	539	GLY	CA-C-N	7.27	131.36	120.31
1	C	539	GLY	C-N-CA	7.27	131.36	120.31
1	A	120	PRO	O-C-N	-7.26	114.34	122.18
2	B	419	GLU	CA-C-N	7.25	129.87	120.44
2	B	419	GLU	C-N-CA	7.25	129.87	120.44
2	B	224	LEU	CA-C-N	7.25	131.32	120.31
2	B	224	LEU	C-N-CA	7.25	131.32	120.31
2	D	48	PRO	CA-C-N	7.24	127.58	119.32
2	D	48	PRO	C-N-CA	7.24	127.58	119.32
1	A	5	PRO	N-CA-CB	7.24	109.75	103.31
2	D	504	SER	CA-C-N	7.24	131.31	120.31
2	D	504	SER	C-N-CA	7.24	131.31	120.31
1	C	185	GLN	CA-C-N	7.23	132.50	121.51
1	C	185	GLN	C-N-CA	7.23	132.50	121.51
1	C	636	THR	N-CA-C	-7.23	99.52	110.07
1	A	526	ASP	CA-C-N	7.22	127.06	119.05
1	A	526	ASP	C-N-CA	7.22	127.06	119.05
1	C	526	ASP	CA-C-O	7.21	127.15	120.09
1	A	484	ASP	CA-CB-CG	-7.20	105.40	112.60
1	C	398	ARG	N-CA-C	7.19	119.98	111.71
1	C	577	THR	CA-C-N	7.17	126.80	119.19
1	C	577	THR	C-N-CA	7.17	126.80	119.19
1	C	535	CYS	O-C-N	-7.17	113.97	122.15
1	C	520	GLY	O-C-N	-7.16	114.47	122.28
2	D	422	GLU	O-C-N	-7.16	114.64	122.09
2	B	439	THR	CA-C-O	-7.16	113.24	120.90
2	D	558	LYS	O-C-N	-7.15	114.71	122.07
1	C	184	GLU	O-C-N	-7.14	113.86	122.22
2	D	251	GLU	CB-CG-CD	7.14	124.74	112.60
2	D	543	PRO	N-CA-CB	7.12	109.55	103.35
2	B	93	PHE	CA-C-N	7.12	130.15	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	PHE	C-N-CA	7.12	130.15	120.54
2	B	600	LYS	O-C-N	-7.12	112.89	122.43
1	A	405	GLY	O-C-N	-7.11	114.98	122.52
1	C	466	GLY	O-C-N	-7.11	113.10	122.42
1	A	272	SER	O-C-N	-7.11	113.14	122.39
2	B	228	SER	CA-C-N	7.11	126.74	119.56
2	B	228	SER	C-N-CA	7.11	126.74	119.56
2	D	521	ARG	CA-C-N	7.10	129.80	120.28
2	D	521	ARG	C-N-CA	7.10	129.80	120.28
1	C	52	GLU	N-CA-C	7.10	121.39	112.87
1	C	430	VAL	O-C-N	-7.10	113.70	122.57
1	A	726	LEU	N-CA-C	7.09	121.04	112.38
1	C	189	PRO	CA-C-N	7.09	131.09	120.31
1	C	189	PRO	C-N-CA	7.09	131.09	120.31
2	D	521	ARG	O-C-N	-7.09	114.60	122.12
2	D	333	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	A	149	MET	CA-C-N	7.08	129.77	120.28
1	A	149	MET	C-N-CA	7.08	129.77	120.28
1	C	282	PRO	O-C-N	-7.07	112.76	122.24
1	C	477	PRO	N-CA-CB	7.07	109.50	103.35
2	B	180	VAL	N-CA-CB	7.07	121.18	110.58
1	A	678	PRO	CA-C-O	7.07	128.00	118.81
1	A	232	MET	CA-C-N	7.07	126.77	119.56
1	A	232	MET	C-N-CA	7.07	126.77	119.56
2	B	273	ALA	CA-C-N	7.06	129.75	120.28
2	B	273	ALA	C-N-CA	7.06	129.75	120.28
1	C	120	PRO	O-C-N	-7.05	114.20	122.17
1	A	690	GLU	O-C-N	-7.04	113.98	122.22
1	C	672	LEU	CA-C-N	7.04	129.71	120.28
1	C	672	LEU	C-N-CA	7.04	129.71	120.28
2	D	286	ALA	N-CA-C	-7.04	97.05	108.52
1	C	379	SER	O-C-N	-7.03	114.67	122.12
1	C	498	LYS	CA-C-N	7.03	130.03	120.54
1	C	498	LYS	C-N-CA	7.03	130.03	120.54
1	A	627	ASP	N-CA-C	-7.03	97.79	108.96
1	C	89	TYR	CA-CB-CG	7.01	126.52	113.90
1	A	123	ARG	CA-C-N	7.01	135.14	121.41
1	A	123	ARG	C-N-CA	7.01	135.14	121.41
2	B	422	GLU	CA-C-N	7.01	130.06	120.46
2	B	422	GLU	C-N-CA	7.01	130.06	120.46
1	A	448	GLU	CA-C-N	7.00	129.66	120.28
1	A	448	GLU	C-N-CA	7.00	129.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	PRO	N-CA-CB	7.00	109.54	103.31
1	A	183	GLU	O-C-N	-6.99	114.07	122.11
1	C	574	VAL	N-CA-CB	6.99	122.77	111.23
1	A	129	ASN	CA-C-N	6.99	126.81	119.05
1	A	129	ASN	C-N-CA	6.99	126.81	119.05
2	D	613	ILE	CA-C-O	6.99	128.61	120.71
2	B	352	VAL	CA-C-N	6.98	136.76	121.19
2	B	352	VAL	C-N-CA	6.98	136.76	121.19
1	A	175	LEU	CA-C-N	6.98	129.52	120.44
1	A	175	LEU	C-N-CA	6.98	129.52	120.44
1	A	333	GLY	CA-C-O	6.98	128.06	120.66
1	A	500	ARG	CA-C-N	6.98	129.93	120.44
1	A	500	ARG	C-N-CA	6.98	129.93	120.44
2	D	266	LEU	CA-C-N	6.98	130.33	120.42
2	D	266	LEU	C-N-CA	6.98	130.33	120.42
2	B	550	THR	CA-C-N	6.95	129.48	120.44
2	B	550	THR	C-N-CA	6.95	129.48	120.44
1	C	665	VAL	O-C-N	-6.95	115.97	120.42
2	D	393	GLY	CA-C-N	6.94	133.29	121.14
2	D	393	GLY	C-N-CA	6.94	133.29	121.14
1	A	300	LYS	O-C-N	-6.94	114.87	122.09
1	A	224	ILE	O-C-N	-6.94	114.69	121.83
1	C	333	GLY	CA-C-O	6.93	128.01	120.66
1	A	711	ILE	CA-C-N	6.92	127.21	119.32
1	A	711	ILE	C-N-CA	6.92	127.21	119.32
2	B	340	ILE	N-CA-CB	6.92	118.65	110.55
2	D	398	PRO	O-C-N	-6.91	113.31	122.22
1	A	262	ASP	O-C-N	-6.90	114.80	122.12
2	B	521	ARG	CA-C-N	6.90	129.83	120.38
2	B	521	ARG	C-N-CA	6.90	129.83	120.38
1	A	256	MET	CB-CA-C	-6.90	100.05	110.88
1	C	334	TRP	O-C-N	-6.90	114.81	122.12
2	B	362	PRO	N-CA-CB	6.90	109.35	103.35
1	A	488	VAL	N-CA-CB	6.89	119.39	110.57
2	D	577	GLN	N-CA-C	6.89	121.86	113.38
1	A	44	ILE	N-CA-C	-6.89	99.88	107.73
2	B	556	ALA	O-C-N	-6.89	114.92	122.09
2	B	604	ASP	CA-C-N	6.88	135.71	121.94
2	B	604	ASP	C-N-CA	6.88	135.71	121.94
1	A	434	ALA	CA-C-N	6.88	129.49	120.28
1	A	434	ALA	C-N-CA	6.88	129.49	120.28
1	A	548	MET	CA-C-N	6.87	130.75	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	MET	C-N-CA	6.87	130.75	120.31
2	B	77	ARG	CA-C-N	6.87	127.15	119.32
2	B	77	ARG	C-N-CA	6.87	127.15	119.32
1	C	30	ALA	CA-C-N	6.87	130.75	120.31
1	C	30	ALA	C-N-CA	6.87	130.75	120.31
1	C	313	HIS	CA-C-N	6.87	131.68	120.63
1	C	313	HIS	C-N-CA	6.87	131.68	120.63
2	B	608	GLU	CA-C-N	6.86	129.80	120.54
2	B	608	GLU	C-N-CA	6.86	129.80	120.54
1	A	357	GLN	O-C-N	-6.86	113.00	122.46
1	C	145	SER	CA-C-N	6.85	130.19	120.53
1	C	145	SER	C-N-CA	6.85	130.19	120.53
1	A	507	LYS	CA-C-N	6.85	129.19	120.56
1	A	507	LYS	C-N-CA	6.85	129.19	120.56
1	A	334	TRP	CA-C-N	6.84	132.14	120.72
1	A	334	TRP	C-N-CA	6.84	132.14	120.72
2	B	374	PHE	CA-C-N	6.84	126.64	119.05
2	B	374	PHE	C-N-CA	6.84	126.64	119.05
1	A	209	THR	N-CA-CB	6.84	121.45	111.54
2	B	617	LEU	N-CA-CB	6.83	121.31	110.65
1	A	107	ALA	O-C-N	-6.83	114.23	122.22
1	A	449	ALA	O-C-N	-6.83	114.88	122.12
1	C	314	GLN	O-C-N	-6.82	113.46	122.33
1	A	101	PHE	O-C-N	-6.82	115.05	122.07
1	C	371	ALA	CA-C-N	6.81	129.92	122.77
1	C	371	ALA	C-N-CA	6.81	129.92	122.77
2	B	497	PHE	CA-CB-CG	-6.81	106.99	113.80
1	C	129	ASN	CA-C-O	6.81	126.23	119.49
1	A	184	GLU	CA-C-N	6.81	135.55	121.94
1	A	184	GLU	C-N-CA	6.81	135.55	121.94
1	C	184	GLU	CA-C-N	6.80	134.85	121.58
1	C	184	GLU	C-N-CA	6.80	134.85	121.58
2	D	95	ARG	CG-CD-NE	6.80	126.97	112.00
2	B	466	PHE	O-C-N	-6.80	118.40	121.53
1	C	526	ASP	CA-C-N	6.80	127.07	119.32
1	C	526	ASP	C-N-CA	6.80	127.07	119.32
1	A	527	PRO	CA-C-N	6.79	131.47	120.60
1	A	527	PRO	C-N-CA	6.79	131.47	120.60
2	D	533	PRO	N-CA-CB	6.79	110.73	103.39
2	D	423	VAL	CA-C-N	6.79	129.27	120.44
2	D	423	VAL	C-N-CA	6.79	129.27	120.44
2	B	634	LEU	CA-C-N	6.78	134.89	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	634	LEU	C-N-CA	6.78	134.89	121.53
1	C	222	SER	O-C-N	-6.78	114.47	122.20
2	D	200	ASP	CA-C-N	6.78	126.58	119.05
2	D	200	ASP	C-N-CA	6.78	126.58	119.05
2	B	79	LYS	CA-C-N	6.78	134.80	121.58
2	B	79	LYS	C-N-CA	6.78	134.80	121.58
2	B	75	MET	O-C-N	-6.78	115.38	123.31
1	C	97	GLU	CA-C-N	6.78	129.25	120.44
1	C	97	GLU	C-N-CA	6.78	129.25	120.44
1	C	727	ASP	CA-C-N	6.77	133.89	121.70
1	C	727	ASP	C-N-CA	6.77	133.89	121.70
1	A	421	TRP	CA-C-N	6.77	127.50	119.98
1	A	421	TRP	C-N-CA	6.77	127.50	119.98
1	C	123	ARG	CA-C-N	6.77	133.46	120.66
1	C	123	ARG	C-N-CA	6.77	133.46	120.66
1	C	243	TYR	CA-C-N	6.77	129.35	120.28
1	C	243	TYR	C-N-CA	6.77	129.35	120.28
2	D	259	GLY	CA-C-N	6.76	129.64	120.38
2	D	259	GLY	C-N-CA	6.76	129.64	120.38
1	C	28	LEU	CA-C-N	6.76	129.23	120.44
1	C	28	LEU	C-N-CA	6.76	129.23	120.44
2	B	127	GLU	CA-C-N	6.76	127.48	119.98
2	B	127	GLU	C-N-CA	6.76	127.48	119.98
2	B	146	ALA	CA-C-N	6.76	127.31	119.47
2	B	146	ALA	C-N-CA	6.76	127.31	119.47
1	C	553	GLU	O-C-N	-6.75	114.96	122.12
2	B	301	ARG	CA-C-O	-6.75	113.39	120.55
1	C	550	ASP	CA-C-N	6.75	129.63	120.38
1	C	550	ASP	C-N-CA	6.75	129.63	120.38
1	A	528	ASP	CA-C-N	6.74	133.92	122.26
1	A	528	ASP	C-N-CA	6.74	133.92	122.26
1	C	272	SER	O-C-N	-6.73	113.58	122.33
1	A	388	LEU	CA-C-N	6.73	129.19	120.44
1	A	388	LEU	C-N-CA	6.73	129.19	120.44
1	C	666	PRO	N-CA-CB	6.73	110.73	103.33
2	D	349	SER	CA-C-N	6.73	129.59	120.44
2	D	349	SER	C-N-CA	6.73	129.59	120.44
2	D	84	LYS	CA-C-O	-6.73	113.10	120.43
1	A	593	ALA	O-C-N	-6.73	114.48	122.15
1	C	469	LYS	CA-C-N	6.73	131.69	122.34
1	C	469	LYS	C-N-CA	6.73	131.69	122.34
1	A	177	LEU	O-C-N	-6.72	114.36	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	GLN	CA-C-N	6.72	126.51	119.05
1	C	215	GLN	C-N-CA	6.72	126.51	119.05
1	C	277	VAL	O-C-N	-6.71	115.31	121.89
2	D	605	ASP	CA-C-N	6.71	129.60	120.54
2	D	605	ASP	C-N-CA	6.71	129.60	120.54
1	C	469	LYS	O-C-N	-6.71	115.77	123.42
2	D	532	SER	CA-C-N	6.71	126.66	119.28
2	D	532	SER	C-N-CA	6.71	126.66	119.28
1	C	17	VAL	N-CA-C	-6.71	100.08	107.73
1	C	535	CYS	CA-C-N	6.70	129.65	120.46
1	C	535	CYS	C-N-CA	6.70	129.65	120.46
2	D	424	GLU	CA-C-N	6.70	129.26	120.28
2	D	424	GLU	C-N-CA	6.70	129.26	120.28
2	B	477	LYS	N-CA-C	-6.70	101.34	109.72
1	A	541	ALA	CA-C-N	6.70	134.33	121.54
1	A	541	ALA	C-N-CA	6.70	134.33	121.54
1	C	150	ARG	CA-C-N	6.70	129.80	120.29
1	C	150	ARG	C-N-CA	6.70	129.80	120.29
1	C	727	ASP	CA-CB-CG	6.69	119.29	112.60
2	B	88	PRO	N-CA-CB	6.69	109.55	103.33
1	A	499	LEU	CA-C-N	6.69	129.24	120.28
1	A	499	LEU	C-N-CA	6.69	129.24	120.28
2	D	232	ARG	CD-NE-CZ	6.69	133.76	124.40
2	D	390	VAL	CA-C-O	6.68	126.91	119.42
1	C	430	VAL	CA-CB-CG1	6.68	121.76	110.40
2	D	529	GLY	CA-C-N	6.68	131.71	120.88
2	D	529	GLY	C-N-CA	6.68	131.71	120.88
2	B	79	LYS	O-C-N	-6.67	113.71	122.39
1	A	189	PRO	CA-C-N	6.67	131.86	120.72
1	A	189	PRO	C-N-CA	6.67	131.86	120.72
2	D	511	PRO	N-CA-CB	6.67	109.15	103.35
1	A	304	ALA	O-C-N	-6.66	115.06	122.12
2	D	397	ASP	CA-CB-CG	6.66	119.26	112.60
2	B	604	ASP	O-C-N	-6.66	114.43	122.22
1	A	608	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	636	THR	N-CA-C	-6.65	100.36	110.07
2	B	328	TRP	CA-C-N	6.65	129.49	120.38
2	B	328	TRP	C-N-CA	6.65	129.49	120.38
1	A	430	VAL	CA-CB-CG1	6.65	121.70	110.40
2	B	73	VAL	CA-C-N	6.65	126.24	119.19
2	B	73	VAL	C-N-CA	6.65	126.24	119.19
2	D	77	ARG	CA-C-N	6.65	126.90	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	77	ARG	C-N-CA	6.65	126.90	119.32
2	B	432	ALA	CA-C-N	6.64	129.85	120.42
2	B	432	ALA	C-N-CA	6.64	129.85	120.42
1	C	707	PRO	N-CA-CB	6.64	109.10	103.25
1	A	345	VAL	CA-C-N	6.63	129.05	120.56
1	A	345	VAL	C-N-CA	6.63	129.05	120.56
1	A	439	LYS	O-C-N	-6.63	113.61	122.43
1	A	189	PRO	O-C-N	-6.63	114.62	122.24
1	C	488	VAL	N-CA-CB	6.63	119.05	110.57
2	B	529	GLY	CA-C-N	6.62	131.77	120.71
2	B	529	GLY	C-N-CA	6.62	131.77	120.71
1	C	188	LYS	CA-C-N	6.62	127.15	119.47
1	C	188	LYS	C-N-CA	6.62	127.15	119.47
2	B	523	ASP	CB-CA-C	-6.62	100.44	110.90
2	D	278	ASP	CA-C-N	6.62	132.11	121.98
2	D	278	ASP	C-N-CA	6.62	132.11	121.98
1	A	231	ASN	N-CA-C	6.62	122.32	113.72
2	D	123	LYS	CA-C-N	6.61	129.46	120.54
2	D	123	LYS	C-N-CA	6.61	129.46	120.54
2	B	455	ASN	CA-CB-CG	6.61	119.21	112.60
1	C	59	ASP	CA-CB-CG	6.61	119.21	112.60
2	B	25	GLY	CA-C-N	6.61	134.46	121.58
2	B	25	GLY	C-N-CA	6.61	134.46	121.58
1	A	282	PRO	CA-C-N	6.60	132.89	122.60
1	A	282	PRO	C-N-CA	6.60	132.89	122.60
2	D	397	ASP	CA-C-N	6.59	126.53	119.28
2	D	397	ASP	C-N-CA	6.59	126.53	119.28
2	D	304	TRP	O-C-N	-6.59	115.24	122.09
1	C	232	MET	CA-C-N	6.59	126.22	119.56
1	C	232	MET	C-N-CA	6.59	126.22	119.56
2	D	531	SER	N-CA-C	6.59	118.12	111.07
1	C	262	ASP	N-CA-CB	6.59	119.56	110.01
1	A	601	LEU	N-CA-C	-6.58	98.51	109.24
2	D	462	ALA	O-C-N	-6.58	113.77	122.00
1	A	70	PHE	O-C-N	-6.58	113.78	122.40
1	A	153	PHE	CA-CB-CG	-6.58	107.22	113.80
1	A	281	ALA	N-CA-CB	6.58	120.10	110.30
1	C	633	LEU	CA-C-N	6.57	133.37	123.05
1	C	633	LEU	C-N-CA	6.57	133.37	123.05
2	D	297	LEU	CA-C-N	6.57	129.61	120.29
2	D	297	LEU	C-N-CA	6.57	129.61	120.29
2	D	308	GLY	CA-C-N	6.57	129.08	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	308	GLY	C-N-CA	6.57	129.08	120.28
2	D	558	LYS	CA-C-N	6.56	129.08	120.28
2	D	558	LYS	C-N-CA	6.56	129.08	120.28
2	D	460	ILE	N-CA-CB	6.56	120.17	111.64
1	C	332	SER	CA-C-O	6.55	128.18	120.58
1	C	70	PHE	O-C-N	-6.55	113.88	122.59
1	C	253	ASP	CA-C-N	6.54	128.94	120.56
1	C	253	ASP	C-N-CA	6.54	128.94	120.56
1	C	699	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	344	ASN	O-C-N	-6.54	114.57	122.22
2	B	59	LEU	CA-C-N	6.54	129.37	120.54
2	B	59	LEU	C-N-CA	6.54	129.37	120.54
1	A	468	ASN	CA-CB-CG	6.54	119.14	112.60
2	B	408	LEU	CA-C-N	6.54	128.94	120.44
2	B	408	LEU	C-N-CA	6.54	128.94	120.44
2	D	23	LEU	O-C-N	-6.54	113.90	122.59
1	A	271	GLU	CA-C-N	6.53	131.05	120.60
1	A	271	GLU	C-N-CA	6.53	131.05	120.60
1	C	63	THR	O-C-N	-6.53	113.89	122.97
2	D	79	LYS	O-C-N	-6.53	113.91	122.39
2	D	82	PRO	N-CA-CB	6.53	109.03	103.35
1	C	677	ARG	CA-C-N	6.52	126.23	119.64
1	C	677	ARG	C-N-CA	6.52	126.23	119.64
2	B	435	THR	O-C-N	-6.52	113.92	122.59
2	B	239	ASN	O-C-N	-6.52	114.59	122.22
1	A	312	VAL	O-C-N	-6.51	114.44	121.80
2	D	404	TYR	CA-C-O	-6.51	113.91	121.07
1	C	684	VAL	N-CA-CB	6.51	121.02	111.52
2	D	347	THR	O-C-N	-6.50	115.23	122.12
1	A	219	ARG	O-C-N	-6.50	115.23	122.12
2	B	390	VAL	O-C-N	-6.50	114.51	122.18
1	C	264	VAL	O-C-N	-6.50	115.54	121.91
2	B	337	TYR	CA-C-N	6.50	130.73	120.47
2	B	337	TYR	C-N-CA	6.50	130.73	120.47
1	C	521	ASN	O-C-N	-6.49	115.45	121.36
1	A	122	HIS	CA-CB-CG	-6.49	107.31	113.80
2	D	79	LYS	CA-C-N	6.49	134.23	121.58
2	D	79	LYS	C-N-CA	6.49	134.23	121.58
2	B	632	ASP	O-C-N	-6.49	115.14	122.08
1	C	593	ALA	O-C-N	-6.48	114.76	122.15
1	C	253	ASP	CA-CB-CG	6.48	119.08	112.60
2	B	141	ASP	CA-C-N	6.47	126.24	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	ASP	C-N-CA	6.47	126.24	119.05
1	A	277	VAL	CA-C-N	6.47	130.96	120.60
1	A	277	VAL	C-N-CA	6.47	130.96	120.60
1	A	539	GLY	CA-C-N	6.47	129.48	120.29
1	A	539	GLY	C-N-CA	6.47	129.48	120.29
2	D	273	ALA	N-CA-C	-6.47	103.73	111.69
1	A	379	SER	O-C-N	-6.47	115.27	122.12
1	A	411	GLU	CA-C-N	6.46	128.94	120.28
1	A	411	GLU	C-N-CA	6.46	128.94	120.28
1	A	244	HIS	CA-C-N	6.46	128.94	120.28
1	A	244	HIS	C-N-CA	6.46	128.94	120.28
1	A	105	ASN	CA-C-N	6.46	128.84	120.44
1	A	105	ASN	C-N-CA	6.46	128.84	120.44
1	A	626	PHE	CA-CB-CG	6.46	120.26	113.80
2	B	59	LEU	O-C-N	-6.46	115.42	122.07
1	C	439	LYS	CA-C-N	6.45	132.62	121.07
1	C	439	LYS	C-N-CA	6.45	132.62	121.07
2	B	204	PHE	CA-C-N	6.45	128.83	120.44
2	B	204	PHE	C-N-CA	6.45	128.83	120.44
2	B	203	GLY	CA-C-N	6.45	128.82	120.44
2	B	203	GLY	C-N-CA	6.45	128.82	120.44
1	A	667	ALA	CA-C-N	6.44	129.44	120.29
1	A	667	ALA	C-N-CA	6.44	129.44	120.29
1	A	63	THR	CA-C-N	6.44	132.60	122.94
1	A	63	THR	C-N-CA	6.44	132.60	122.94
1	A	213	PRO	CA-C-N	6.44	125.94	119.24
1	A	213	PRO	C-N-CA	6.44	125.94	119.24
2	B	212	PRO	N-CA-CB	6.44	108.90	103.17
2	D	141	ASP	CA-C-N	6.43	125.66	118.97
2	D	141	ASP	C-N-CA	6.43	125.66	118.97
1	A	18	PRO	N-CA-CB	6.43	109.44	103.39
1	C	304	ALA	CA-C-O	-6.43	113.73	120.55
1	C	527	PRO	N-CA-CB	6.43	110.59	103.26
2	B	56	ALA	CA-C-N	6.43	129.18	120.44
2	B	56	ALA	C-N-CA	6.43	129.18	120.44
1	A	673	ASP	CA-C-N	6.42	129.76	120.38
1	A	673	ASP	C-N-CA	6.42	129.76	120.38
2	B	390	VAL	CA-C-O	6.42	126.61	119.42
2	D	633	ILE	O-C-N	-6.42	115.60	121.89
1	C	101	PHE	O-C-N	-6.41	115.32	122.12
1	A	665	VAL	CA-C-N	6.40	125.62	118.97
1	A	665	VAL	C-N-CA	6.40	125.62	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	PHE	CA-CB-CG	-6.40	107.40	113.80
2	D	20	THR	CA-C-N	-6.39	114.27	122.77
2	D	20	THR	C-N-CA	-6.39	114.27	122.77
1	C	595	GLY	O-C-N	-6.39	114.97	122.45
2	D	536	HIS	CA-C-N	6.39	128.84	120.60
2	D	536	HIS	C-N-CA	6.39	128.84	120.60
1	C	107	ALA	CA-C-N	6.39	133.55	122.56
1	C	107	ALA	C-N-CA	6.39	133.55	122.56
1	A	233	PRO	N-CA-CB	6.38	109.86	103.48
1	A	683	THR	N-CA-CB	6.38	121.99	111.08
1	A	694	ASP	CA-C-N	6.38	128.83	120.28
1	A	694	ASP	C-N-CA	6.38	128.83	120.28
2	D	73	VAL	CA-C-N	6.38	125.95	119.19
2	D	73	VAL	C-N-CA	6.38	125.95	119.19
1	A	260	LEU	O-C-N	-6.37	114.88	122.15
2	B	455	ASN	CA-C-N	6.37	131.64	122.40
2	B	455	ASN	C-N-CA	6.37	131.64	122.40
1	C	591	GLU	CA-C-N	6.37	129.13	120.54
1	C	591	GLU	C-N-CA	6.37	129.13	120.54
1	C	617	ILE	CA-C-O	-6.36	114.42	121.17
2	D	397	ASP	CA-C-O	6.36	128.88	120.16
2	D	307	ILE	O-C-N	-6.36	115.09	121.96
2	B	257	ALA	CA-C-N	6.35	129.30	120.29
2	B	257	ALA	C-N-CA	6.35	129.30	120.29
1	A	636	THR	CA-C-N	6.34	126.26	119.28
1	A	636	THR	C-N-CA	6.34	126.26	119.28
1	C	272	SER	CA-C-N	6.34	131.29	122.28
1	C	272	SER	C-N-CA	6.34	131.29	122.28
2	D	327	SER	N-CA-C	6.34	119.41	109.96
2	D	501	MET	O-C-N	-6.34	115.40	122.12
2	B	162	THR	N-CA-C	6.34	119.23	108.90
2	D	335	ASP	CA-C-N	6.34	125.96	119.56
2	D	335	ASP	C-N-CA	6.34	125.96	119.56
1	A	504	ASP	CA-C-N	6.33	125.96	119.56
1	A	504	ASP	C-N-CA	6.33	125.96	119.56
2	D	32	GLU	CA-C-N	6.33	129.06	120.38
2	D	32	GLU	C-N-CA	6.33	129.06	120.38
1	C	30	ALA	O-C-N	-6.33	115.41	122.12
1	A	552	LEU	CA-C-O	6.33	127.01	119.60
2	B	335	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	133	ALA	CA-C-N	6.32	132.05	120.79
1	A	133	ALA	C-N-CA	6.32	132.05	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	677	ARG	O-C-N	-6.32	115.71	121.34
2	D	420	PHE	N-CA-C	-6.32	104.31	111.14
1	C	494	ALA	CA-C-N	6.32	128.75	120.28
1	C	494	ALA	C-N-CA	6.32	128.75	120.28
2	B	327	SER	CA-C-O	6.32	127.97	120.70
2	B	191	LYS	CA-C-N	6.32	133.19	122.26
2	B	191	LYS	C-N-CA	6.32	133.19	122.26
1	A	667	ALA	O-C-N	-6.31	115.43	122.12
1	C	320	PRO	CA-C-N	6.31	129.37	120.28
1	C	320	PRO	C-N-CA	6.31	129.37	120.28
1	A	54	VAL	CA-C-O	-6.31	113.82	120.57
2	D	154	LEU	CA-C-N	6.31	128.73	120.28
2	D	154	LEU	C-N-CA	6.31	128.73	120.28
1	C	300	LYS	O-C-N	-6.30	115.54	122.09
2	D	375	PRO	CA-C-N	6.30	128.72	120.28
2	D	375	PRO	C-N-CA	6.30	128.72	120.28
1	C	497	VAL	N-CA-C	-6.30	104.37	110.42
1	C	369	ASP	O-C-N	-6.30	112.28	122.42
1	A	277	VAL	O-C-N	-6.30	115.76	121.87
1	C	582	GLU	CA-C-N	6.29	128.62	120.44
1	C	582	GLU	C-N-CA	6.29	128.62	120.44
1	C	206	VAL	CA-CB-CG1	6.29	121.09	110.40
2	B	522	ARG	CD-NE-CZ	6.29	133.20	124.40
1	A	586	LEU	O-C-N	-6.28	115.46	122.12
2	B	308	GLY	CA-C-N	6.28	128.70	120.28
2	B	308	GLY	C-N-CA	6.28	128.70	120.28
1	A	183	GLU	CA-C-N	6.28	129.55	120.38
1	A	183	GLU	C-N-CA	6.28	129.55	120.38
2	B	167	PHE	CA-CB-CG	6.28	120.08	113.80
1	C	665	VAL	CA-C-N	6.28	126.02	119.05
1	C	665	VAL	C-N-CA	6.28	126.02	119.05
1	A	146	ILE	O-C-N	-6.28	115.53	121.87
2	B	363	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	63	THR	N-CA-CB	6.27	120.05	110.70
1	A	145	SER	CA-C-N	6.27	130.38	120.47
1	A	145	SER	C-N-CA	6.27	130.38	120.47
1	C	248	ALA	CA-C-N	6.26	133.68	121.41
1	C	248	ALA	C-N-CA	6.26	133.68	121.41
1	C	263	GLY	O-C-N	-6.25	116.19	122.19
2	B	298	ARG	CD-NE-CZ	6.25	133.15	124.40
2	B	401	GLY	O-C-N	-6.25	115.59	122.65
2	D	338	VAL	CA-C-N	6.25	129.28	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	VAL	C-N-CA	6.25	129.28	120.28
2	B	375	PRO	N-CA-CB	6.25	110.20	103.33
1	C	310	LYS	CA-C-N	6.24	128.64	120.28
1	C	310	LYS	C-N-CA	6.24	128.64	120.28
1	C	131	ARG	N-CA-C	6.24	119.99	112.38
2	D	224	LEU	CA-C-N	6.24	129.79	120.31
2	D	224	LEU	C-N-CA	6.24	129.79	120.31
1	A	652	VAL	N-CA-CB	6.23	119.52	111.67
1	A	60	TRP	CA-C-N	6.23	130.57	120.60
1	A	60	TRP	C-N-CA	6.23	130.57	120.60
1	C	413	THR	CA-C-N	6.23	128.54	120.44
1	C	413	THR	C-N-CA	6.23	128.54	120.44
2	D	352	VAL	O-C-N	-6.23	114.76	121.80
1	C	385	ASN	CA-C-N	6.23	128.95	120.54
1	C	385	ASN	C-N-CA	6.23	128.95	120.54
1	C	663	THR	N-CA-C	-6.22	105.34	113.12
2	D	258	THR	CA-C-N	6.22	126.85	119.94
2	D	258	THR	C-N-CA	6.22	126.85	119.94
1	A	429	LYS	O-C-N	-6.22	115.53	122.12
2	D	283	ARG	N-CA-CB	6.22	120.64	110.37
2	D	292	LEU	N-CA-C	-6.22	104.04	111.69
2	D	425	LYS	CA-C-N	6.22	133.70	121.58
2	D	425	LYS	C-N-CA	6.22	133.70	121.58
1	C	6	ARG	CD-NE-CZ	6.21	133.10	124.40
1	C	269	ALA	O-C-N	-6.21	115.53	122.12
2	D	532	SER	O-C-N	-6.21	114.17	121.32
2	D	191	LYS	CA-C-N	6.21	133.21	122.09
2	D	191	LYS	C-N-CA	6.21	133.21	122.09
1	A	320	PRO	CA-C-N	6.21	129.22	120.28
1	A	320	PRO	C-N-CA	6.21	129.22	120.28
1	A	188	LYS	CA-C-N	6.20	126.39	119.32
1	A	188	LYS	C-N-CA	6.20	126.39	119.32
1	A	104	ARG	CA-C-N	6.20	128.87	120.44
1	A	104	ARG	C-N-CA	6.20	128.87	120.44
2	D	180	VAL	N-CA-CB	6.20	119.88	110.58
2	D	478	PRO	N-CA-CB	6.20	108.75	103.35
2	B	599	PHE	CA-C-N	6.20	131.07	120.72
2	B	599	PHE	C-N-CA	6.20	131.07	120.72
1	A	527	PRO	N-CA-CB	6.19	110.14	103.33
2	B	483	PRO	N-CA-CB	6.19	108.84	103.27
2	D	429	MET	N-CA-C	6.19	118.03	111.28
1	A	225	PHE	CA-CB-CG	6.19	119.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	THR	O-C-N	-6.19	115.73	122.79
1	C	295	PHE	CA-CB-CG	-6.19	107.61	113.80
1	C	405	GLY	O-C-N	-6.18	116.22	122.65
1	C	587	VAL	CA-C-N	6.18	128.57	120.28
1	C	587	VAL	C-N-CA	6.18	128.57	120.28
1	A	622	ALA	CA-C-N	6.18	131.04	120.72
1	A	622	ALA	C-N-CA	6.18	131.04	120.72
2	B	55	PHE	CA-CB-CG	-6.18	107.62	113.80
1	C	428	GLU	CA-C-N	6.18	129.70	120.31
1	C	428	GLU	C-N-CA	6.18	129.70	120.31
1	C	504	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	264	VAL	CA-C-N	6.18	128.56	120.28
1	C	264	VAL	C-N-CA	6.18	128.56	120.28
1	C	593	ALA	CA-C-O	-6.18	113.87	120.42
1	A	521	ASN	O-C-N	-6.17	115.74	121.36
1	C	381	ARG	O-C-N	-6.17	115.11	122.15
2	B	460	ILE	N-CA-CB	6.17	120.00	112.10
1	A	445	ARG	O-C-N	-6.17	115.72	122.07
1	C	513	ASP	O-C-N	-6.17	115.58	122.12
2	D	57	GLU	O-C-N	-6.17	115.72	122.07
2	B	147	PRO	O-C-N	-6.16	114.71	122.17
2	B	218	GLY	O-C-N	-6.16	116.19	122.17
1	A	617	ILE	CA-C-O	-6.16	114.55	120.95
2	B	95	ARG	CG-CD-NE	6.16	125.55	112.00
1	A	342	TYR	O-C-N	-6.16	113.97	122.46
1	C	211	ILE	CA-C-O	6.16	128.47	120.78
1	C	66	GLY	O-C-N	-6.15	114.72	122.41
2	B	337	TYR	O-C-N	-6.14	115.03	122.22
2	B	420	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	477	PRO	N-CA-CB	6.14	108.78	103.31
2	D	496	VAL	O-C-N	-6.14	115.92	121.87
1	A	677	ARG	O-C-N	-6.13	116.34	121.12
2	D	294	ILE	CA-C-N	6.13	128.49	120.28
2	D	294	ILE	C-N-CA	6.13	128.49	120.28
1	C	429	LYS	CA-C-N	6.12	133.00	121.97
1	C	429	LYS	C-N-CA	6.12	133.00	121.97
2	D	84	LYS	N-CA-C	-6.12	99.26	109.24
1	A	392	GLN	N-CA-C	6.12	120.95	112.45
2	D	420	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	78	MET	O-C-N	-6.12	114.46	122.59
1	A	357	GLN	CA-C-O	6.12	126.89	119.31
2	B	255	ALA	N-CA-C	-6.11	104.54	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	GLU	O-C-N	-6.11	115.64	122.12
1	C	589	GLU	CA-C-N	6.11	128.38	120.44
1	C	589	GLU	C-N-CA	6.11	128.38	120.44
2	B	480	PRO	N-CA-CB	6.11	108.74	103.31
1	C	589	GLU	O-C-N	-6.11	115.19	122.15
1	C	104	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	D	610	GLU	CA-C-N	6.10	128.46	120.28
2	D	610	GLU	C-N-CA	6.10	128.46	120.28
1	C	20	ASP	CA-C-N	6.10	129.27	120.79
1	C	20	ASP	C-N-CA	6.10	129.27	120.79
1	C	118	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	17	VAL	N-CA-C	-6.10	100.94	107.77
1	A	19	ALA	CA-C-N	6.10	132.54	122.73
1	A	19	ALA	C-N-CA	6.10	132.54	122.73
1	A	447	GLU	O-C-N	-6.09	115.09	122.22
1	A	632	PRO	N-CA-CB	6.09	109.00	103.33
2	D	500	LEU	N-CA-C	-6.09	104.72	111.36
1	A	504	ASP	CA-C-O	6.09	123.25	119.29
1	A	82	ARG	CD-NE-CZ	6.08	132.92	124.40
1	A	612	ARG	CA-C-N	6.08	126.57	119.94
1	A	612	ARG	C-N-CA	6.08	126.57	119.94
2	D	184	GLU	CA-C-N	6.08	134.10	121.94
2	D	184	GLU	C-N-CA	6.08	134.10	121.94
2	B	286	ALA	N-CA-C	-6.08	98.61	108.52
1	A	506	GLU	CA-C-N	6.08	128.75	120.54
1	A	506	GLU	C-N-CA	6.08	128.75	120.54
1	C	82	ARG	CD-NE-CZ	6.08	132.91	124.40
1	C	723	ARG	O-C-N	-6.07	115.81	122.07
1	C	63	THR	CA-C-O	6.07	129.55	121.78
2	D	566	ASP	CA-CB-CG	6.07	118.67	112.60
2	B	335	ASP	CA-C-N	6.07	125.62	119.19
2	B	335	ASP	C-N-CA	6.07	125.62	119.19
1	C	344	ASN	O-C-N	-6.07	115.12	122.22
2	B	28	PRO	N-CA-CB	6.07	108.71	103.31
2	D	457	LYS	O-C-N	-6.05	113.59	122.43
1	C	198	ASN	O-C-N	-6.05	115.01	122.57
1	A	211	ILE	N-CA-CB	6.04	121.19	111.23
1	A	454	GLN	O-C-N	-6.04	115.72	122.12
1	C	401	ASP	CA-C-N	6.03	125.92	119.28
1	C	401	ASP	C-N-CA	6.03	125.92	119.28
1	A	231	ASN	O-C-N	-6.03	114.93	122.35
2	D	223	ARG	CD-NE-CZ	6.03	132.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	GLN	CA-C-N	6.02	125.73	119.05
1	A	215	GLN	C-N-CA	6.02	125.73	119.05
2	D	222	ARG	CA-C-N	6.02	128.35	120.28
2	D	222	ARG	C-N-CA	6.02	128.35	120.28
2	B	78	PRO	N-CA-CB	6.02	110.12	103.26
2	B	605	ASP	CA-C-N	6.02	128.66	120.54
2	B	605	ASP	C-N-CA	6.02	128.66	120.54
1	C	466	GLY	CA-C-O	6.02	125.66	119.10
2	B	183	TYR	CA-C-N	6.01	128.34	120.28
2	B	183	TYR	C-N-CA	6.01	128.34	120.28
1	A	320	PRO	N-CA-CB	6.01	109.88	103.39
2	B	116	PRO	N-CA-CB	6.01	109.66	103.23
2	B	255	ALA	CA-C-N	6.01	128.34	120.28
2	B	255	ALA	C-N-CA	6.01	128.34	120.28
2	B	200	ASP	CA-C-N	6.01	125.22	118.97
2	B	200	ASP	C-N-CA	6.01	125.22	118.97
1	C	319	ASN	OD1-CG-ND2	-6.01	116.59	122.60
2	B	128	GLY	O-C-N	-6.00	116.42	122.19
2	B	364	THR	CA-C-N	6.00	130.21	120.60
2	B	364	THR	C-N-CA	6.00	130.21	120.60
2	D	407	SER	O-C-N	-6.00	115.76	122.12
2	B	75	MET	CA-C-O	6.00	126.98	120.32
1	C	637	PRO	O-C-N	-6.00	114.48	122.22
2	D	418	LYS	CA-C-N	6.00	130.88	120.68
2	D	418	LYS	C-N-CA	6.00	130.88	120.68
2	D	228	SER	CA-C-N	6.00	127.11	120.45
2	D	228	SER	C-N-CA	6.00	127.11	120.45
1	C	548	MET	CA-C-O	-6.00	114.19	120.55
2	B	501	MET	O-C-N	-6.00	115.76	122.12
1	A	7	PHE	N-CA-C	5.99	120.43	113.18
2	B	610	GLU	CA-C-N	5.99	128.31	120.28
2	B	610	GLU	C-N-CA	5.99	128.31	120.28
1	C	183	GLU	CA-C-N	5.99	128.91	120.28
1	C	183	GLU	C-N-CA	5.99	128.91	120.28
2	B	222	ARG	CA-C-N	5.99	128.31	120.28
2	B	222	ARG	C-N-CA	5.99	128.31	120.28
1	C	689	PRO	N-CA-CB	5.99	108.56	103.35
2	B	206	ALA	CA-C-N	5.99	131.62	121.14
2	B	206	ALA	C-N-CA	5.99	131.62	121.14
2	B	241	TYR	CA-C-N	5.99	128.22	120.44
2	B	241	TYR	C-N-CA	5.99	128.22	120.44
2	D	425	LYS	O-C-N	-5.99	115.77	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	VAL	O-C-N	-5.99	114.81	122.17
1	C	357	GLN	CA-C-N	5.99	135.59	121.82
1	C	357	GLN	C-N-CA	5.99	135.59	121.82
2	D	47	ARG	CD-NE-CZ	5.98	132.78	124.40
2	B	291	PHE	CA-C-N	5.98	128.78	120.29
2	B	291	PHE	C-N-CA	5.98	128.78	120.29
2	D	190	ALA	CA-C-N	5.98	132.12	120.99
2	D	190	ALA	C-N-CA	5.98	132.12	120.99
2	D	311	PHE	CA-CB-CG	5.97	119.78	113.80
1	C	269	ALA	CA-C-N	5.97	126.57	120.00
1	C	269	ALA	C-N-CA	5.97	126.57	120.00
2	B	457	LYS	O-C-N	-5.97	114.22	122.46
1	A	163	VAL	CA-C-O	5.96	126.65	120.39
1	C	550	ASP	O-C-N	-5.96	115.35	122.15
2	D	183	TYR	CA-C-N	5.96	129.37	120.31
2	D	183	TYR	C-N-CA	5.96	129.37	120.31
2	D	219	ASP	CA-C-N	5.96	128.55	120.38
2	D	219	ASP	C-N-CA	5.96	128.55	120.38
1	C	251	THR	O-C-N	-5.96	116.05	122.85
2	D	316	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	184	GLU	CA-C-N	5.96	134.23	122.31
2	B	184	GLU	C-N-CA	5.96	134.23	122.31
1	A	51	ASN	CA-C-N	5.96	130.13	120.60
1	A	51	ASN	C-N-CA	5.96	130.13	120.60
2	B	577	GLN	N-CA-C	5.96	120.70	113.38
2	D	604	ASP	CA-C-N	5.96	133.16	122.38
2	D	604	ASP	C-N-CA	5.96	133.16	122.38
2	D	26	ASP	CB-CA-C	-5.95	98.11	109.95
1	A	129	ASN	CA-C-O	5.95	124.77	119.59
2	B	601	GLU	CA-C-O	5.95	126.69	119.38
1	C	627	ASP	N-CA-C	-5.95	98.03	108.20
2	D	351	SER	O-C-N	-5.94	115.82	122.12
1	C	189	PRO	N-CA-CB	5.94	109.96	103.30
2	D	142	PRO	N-CA-CB	5.94	109.59	103.23
2	D	536	HIS	O-C-N	-5.94	114.47	122.43
1	A	469	LYS	CA-C-N	5.93	130.59	122.34
1	A	469	LYS	C-N-CA	5.93	130.59	122.34
2	B	498	GLU	CA-C-N	5.93	128.72	120.29
2	B	498	GLU	C-N-CA	5.93	128.72	120.29
2	D	371	GLU	CA-CB-CG	5.93	125.97	114.10
1	A	622	ALA	O-C-N	-5.93	115.83	122.12
2	D	191	LYS	N-CA-C	5.93	119.98	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	256	LEU	CA-C-N	5.93	129.03	120.79
2	D	256	LEU	C-N-CA	5.93	129.03	120.79
2	D	363	PHE	CA-C-N	5.93	133.80	121.94
2	D	363	PHE	C-N-CA	5.93	133.80	121.94
1	C	664	LEU	N-CA-C	5.93	117.74	111.28
2	B	108	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	129	ASN	CA-C-N	5.93	126.08	119.32
1	C	129	ASN	C-N-CA	5.93	126.08	119.32
1	C	155	GLY	O-C-N	-5.92	114.97	122.32
1	C	246	GLN	O-C-N	-5.92	115.69	122.09
2	B	422	GLU	O-C-N	-5.92	115.93	122.09
2	D	465	GLU	O-C-N	-5.92	116.38	123.31
1	C	78	MET	O-C-N	-5.92	114.72	122.59
2	B	222	ARG	O-C-N	-5.91	115.41	122.15
1	C	651	VAL	CA-C-O	5.91	127.27	120.76
1	A	463	PRO	N-CA-CB	5.91	108.49	103.35
1	A	465	ILE	CA-C-O	5.91	127.99	121.13
2	D	397	ASP	O-C-N	-5.91	114.52	121.32
2	D	435	THR	O-C-N	-5.91	114.73	122.59
2	D	243	ASN	CA-C-O	5.91	126.64	119.49
2	D	418	LYS	O-C-N	-5.91	115.31	122.22
2	B	613	ILE	N-CA-C	5.90	117.08	108.58
1	C	88	GLN	CA-C-N	5.90	129.21	120.95
1	C	88	GLN	C-N-CA	5.90	129.21	120.95
1	A	231	ASN	CB-CA-C	-5.90	99.64	109.55
1	A	368	LEU	CA-C-N	5.90	132.44	122.65
1	A	368	LEU	C-N-CA	5.90	132.44	122.65
2	B	190	ALA	O-C-N	-5.90	115.33	122.11
2	D	431	LYS	O-C-N	-5.90	116.00	122.07
1	A	109	GLY	N-CA-C	5.90	122.89	114.64
1	A	696	LEU	N-CA-CB	5.89	118.88	110.16
2	D	171	ASP	CA-C-O	5.89	128.94	120.51
1	C	556	PHE	N-CA-C	5.89	119.65	112.23
1	C	568	GLY	N-CA-C	5.89	122.99	114.10
1	A	321	LYS	CA-C-N	5.89	128.17	120.28
1	A	321	LYS	C-N-CA	5.89	128.17	120.28
2	B	585	LEU	O-C-N	-5.89	116.01	122.07
1	A	591	GLU	CA-C-N	5.88	128.49	120.54
1	A	591	GLU	C-N-CA	5.88	128.49	120.54
1	C	196	ILE	N-CA-C	-5.88	99.88	108.11
1	A	66	GLY	CA-C-O	5.88	126.30	119.13
1	A	358	GLY	N-CA-C	-5.88	107.62	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	PHE	CA-C-N	5.88	128.43	120.38
2	B	55	PHE	C-N-CA	5.88	128.43	120.38
1	A	152	LEU	O-C-N	-5.87	115.89	122.12
1	C	412	LEU	CA-C-N	5.87	128.07	120.44
1	C	412	LEU	C-N-CA	5.87	128.07	120.44
2	B	338	VAL	CA-C-N	5.87	129.99	120.60
2	B	338	VAL	C-N-CA	5.87	129.99	120.60
2	D	408	LEU	CA-C-N	5.86	128.41	120.44
2	D	408	LEU	C-N-CA	5.86	128.41	120.44
2	D	103	ASP	CA-CB-CG	-5.86	106.74	112.60
1	A	578	PRO	N-CA-CB	5.86	109.72	103.39
1	C	507	LYS	CA-C-N	5.86	128.44	120.77
1	C	507	LYS	C-N-CA	5.86	128.44	120.77
2	B	288	HIS	CA-CB-CG	5.85	119.65	113.80
2	B	443	ASP	CB-CA-C	-5.85	101.08	110.79
1	C	711	ILE	CA-C-N	5.85	125.54	119.05
1	C	711	ILE	C-N-CA	5.85	125.54	119.05
1	A	693	PHE	N-CA-C	5.85	117.65	111.28
1	A	727	ASP	CA-C-N	5.84	132.21	121.70
1	A	727	ASP	C-N-CA	5.84	132.21	121.70
2	D	39	VAL	CA-C-N	5.83	128.42	120.54
2	D	39	VAL	C-N-CA	5.83	128.42	120.54
1	C	74	PRO	CB-CA-C	-5.83	103.59	112.11
1	A	172	LEU	O-C-N	-5.83	115.77	120.38
2	D	115	ASP	CA-CB-CG	5.83	118.43	112.60
2	B	478	PRO	N-CA-CB	5.83	108.22	103.32
2	D	444	ALA	CA-C-N	5.83	128.02	120.44
2	D	444	ALA	C-N-CA	5.83	128.02	120.44
2	B	240	ILE	N-CA-C	-5.83	104.17	110.23
1	A	590	PHE	N-CA-C	-5.82	104.84	111.07
2	D	483	PRO	N-CA-CB	5.82	108.48	103.36
2	D	505	THR	CA-C-N	5.82	128.08	120.28
2	D	505	THR	C-N-CA	5.82	128.08	120.28
2	B	37	ARG	CD-NE-CZ	5.82	132.54	124.40
2	B	521	ARG	O-C-N	-5.82	115.95	122.12
2	D	369	LEU	CA-C-O	5.81	125.83	120.60
1	A	586	LEU	CA-C-N	5.80	128.66	120.42
1	A	586	LEU	C-N-CA	5.80	128.66	120.42
1	C	449	ALA	CA-C-N	5.80	128.52	120.29
1	C	449	ALA	C-N-CA	5.80	128.52	120.29
1	A	123	ARG	O-C-N	-5.80	114.95	122.37
2	B	349	SER	CA-C-N	5.80	127.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	349	SER	C-N-CA	5.80	127.98	120.44
2	B	451	LYS	CA-C-N	5.80	128.05	120.28
2	B	451	LYS	C-N-CA	5.80	128.05	120.28
1	C	287	PHE	CA-CB-CG	5.80	119.60	113.80
2	D	251	GLU	CA-C-N	5.79	128.31	120.44
2	D	251	GLU	C-N-CA	5.79	128.31	120.44
2	D	338	VAL	O-C-N	-5.79	116.02	121.87
2	B	559	LYS	CA-C-N	5.79	128.04	120.28
2	B	559	LYS	C-N-CA	5.79	128.04	120.28
1	A	115	VAL	N-CA-C	5.79	116.64	108.36
1	A	666	PRO	CA-C-N	5.79	128.31	120.38
1	A	666	PRO	C-N-CA	5.79	128.31	120.38
1	C	538	ALA	CA-C-N	5.78	126.40	119.98
1	C	538	ALA	C-N-CA	5.78	126.40	119.98
2	D	93	PHE	CA-C-N	5.78	128.82	120.79
2	D	93	PHE	C-N-CA	5.78	128.82	120.79
2	B	142	PRO	N-CA-CB	5.78	109.68	103.33
2	D	439	THR	O-C-N	-5.78	116.08	122.09
1	C	237	SER	N-CA-C	5.77	120.16	113.18
2	B	270	GLY	N-CA-C	5.77	123.28	115.32
1	C	378	PHE	CA-C-O	-5.77	114.94	121.00
2	D	158	LEU	CA-C-N	5.77	130.35	120.72
2	D	158	LEU	C-N-CA	5.77	130.35	120.72
1	A	601	LEU	N-CA-CB	5.76	119.83	110.43
1	C	377	ASP	CA-CB-CG	5.76	118.36	112.60
2	D	181	SER	CA-C-N	5.76	128.65	120.53
2	D	181	SER	C-N-CA	5.76	128.65	120.53
1	A	376	THR	N-CA-C	-5.76	101.47	110.17
2	B	505	THR	CA-C-N	5.76	129.06	120.31
2	B	505	THR	C-N-CA	5.76	129.06	120.31
1	C	181	THR	CA-C-N	5.76	127.92	120.44
1	C	181	THR	C-N-CA	5.76	127.92	120.44
2	D	223	ARG	O-C-N	-5.76	116.02	122.12
1	C	122	HIS	CA-CB-CG	-5.75	108.05	113.80
1	C	107	ALA	O-C-N	-5.75	115.49	122.22
1	A	300	LYS	CA-C-O	5.75	127.05	120.90
2	B	95	ARG	NE-CZ-NH2	-5.75	114.03	119.20
2	B	185	ARG	CA-C-N	5.75	131.21	122.65
2	B	185	ARG	C-N-CA	5.75	131.21	122.65
2	B	520	THR	O-C-N	-5.74	115.96	122.68
1	A	54	VAL	CA-C-N	5.74	128.55	120.28
1	A	54	VAL	C-N-CA	5.74	128.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	PRO	N-CA-CB	5.74	109.37	103.23
1	A	469	LYS	O-C-N	-5.73	116.89	123.42
1	C	320	PRO	O-C-N	-5.73	114.83	122.22
1	C	683	THR	N-CA-CB	5.73	120.87	111.08
1	C	276	ASN	N-CA-C	-5.72	102.43	110.50
2	D	235	THR	N-CA-CB	5.72	120.19	110.87
2	B	462	ALA	O-C-N	-5.72	114.85	122.00
1	C	720	LYS	CA-C-N	5.72	127.88	120.44
1	C	720	LYS	C-N-CA	5.72	127.88	120.44
1	C	61	LEU	N-CA-C	5.72	122.98	110.80
1	A	527	PRO	O-C-N	-5.72	115.37	122.23
2	B	413	ALA	N-CA-C	-5.72	104.74	110.97
2	D	445	CYS	O-C-N	-5.72	116.18	122.07
1	C	229	SER	CA-C-O	-5.71	114.46	120.63
2	D	305	ALA	O-C-N	-5.71	116.06	122.12
2	D	523	ASP	CA-C-O	-5.71	114.44	120.55
1	A	401	ASP	CA-C-N	5.71	125.83	119.32
1	A	401	ASP	C-N-CA	5.71	125.83	119.32
1	A	353	MET	CA-C-N	5.71	128.20	120.44
1	A	353	MET	C-N-CA	5.71	128.20	120.44
2	B	613	ILE	O-C-N	-5.71	116.44	122.95
2	D	622	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	123	ARG	CD-NE-CZ	5.70	132.38	124.40
2	D	190	ALA	O-C-N	-5.70	115.00	122.59
1	A	506	GLU	N-CA-C	-5.70	104.71	111.03
2	D	124	ALA	CA-C-N	5.70	127.74	120.56
2	D	124	ALA	C-N-CA	5.70	127.74	120.56
2	D	116	PRO	N-CA-CB	5.69	109.32	103.23
2	B	526	GLY	CA-C-N	5.69	127.91	120.28
2	B	526	GLY	C-N-CA	5.69	127.91	120.28
2	D	28	PRO	N-CA-CB	5.69	108.26	103.25
1	A	63	THR	CA-C-O	5.69	129.06	121.78
1	A	70	PHE	N-CA-C	5.69	119.28	111.54
2	D	609	ALA	CA-C-N	5.69	128.18	120.38
2	D	609	ALA	C-N-CA	5.69	128.18	120.38
1	A	390	LEU	O-C-N	-5.69	116.09	122.12
2	B	47	ARG	CD-NE-CZ	5.69	132.36	124.40
1	A	596	ARG	NE-CZ-NH2	-5.69	114.08	119.20
2	D	95	ARG	N-CA-C	5.68	119.31	112.38
1	A	128	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	76	ALA	N-CA-C	5.68	118.20	111.33
1	A	466	GLY	O-C-N	-5.68	114.98	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	610	GLU	O-C-N	-5.68	116.10	122.12
1	C	586	LEU	O-C-N	-5.68	115.68	122.15
2	D	49	PRO	CA-C-N	5.68	131.74	122.65
2	D	49	PRO	C-N-CA	5.68	131.74	122.65
1	A	312	VAL	CA-C-N	5.68	128.16	120.38
1	A	312	VAL	C-N-CA	5.68	128.16	120.38
1	A	133	ALA	O-C-N	-5.67	116.11	122.12
1	A	103	ARG	CD-NE-CZ	5.67	132.34	124.40
2	D	551	ALA	N-CA-C	-5.67	104.79	110.97
1	A	719	VAL	N-CA-C	-5.67	104.80	110.30
1	A	531	LEU	N-CA-C	5.67	117.46	111.28
2	B	47	ARG	CA-C-O	5.67	125.46	120.19
1	C	438	GLU	CA-C-N	5.67	130.18	120.72
1	C	438	GLU	C-N-CA	5.67	130.18	120.72
2	B	416	ALA	CA-C-N	5.66	128.33	120.29
2	B	416	ALA	C-N-CA	5.66	128.33	120.29
2	B	443	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	678	PRO	N-CA-CB	5.66	108.72	103.46
2	B	425	LYS	O-C-N	-5.66	115.60	122.22
2	D	270	GLY	N-CA-C	5.66	122.56	115.21
1	C	411	GLU	O-C-N	-5.66	116.24	122.07
2	D	500	LEU	CA-C-N	5.66	127.86	120.28
2	D	500	LEU	C-N-CA	5.66	127.86	120.28
1	A	715	ALA	CA-C-N	5.65	127.89	120.60
1	A	715	ALA	C-N-CA	5.65	127.89	120.60
1	C	27	GLU	O-C-N	-5.65	116.25	122.07
2	B	187	ASP	CA-CB-CG	5.65	118.25	112.60
2	D	480	PRO	N-CA-CB	5.65	108.33	103.31
1	C	267	ILE	O-C-N	-5.65	116.38	121.91
1	A	717	SER	CA-C-N	5.64	128.30	120.29
1	A	717	SER	C-N-CA	5.64	128.30	120.29
1	A	720	LYS	CA-C-N	5.64	127.78	120.44
1	A	720	LYS	C-N-CA	5.64	127.78	120.44
2	B	87	TYR	CA-C-N	5.64	125.55	119.85
2	B	87	TYR	C-N-CA	5.64	125.55	119.85
2	D	269	GLN	N-CA-C	5.64	122.82	110.80
1	A	314	GLN	CA-C-N	5.64	132.55	122.06
1	A	314	GLN	C-N-CA	5.64	132.55	122.06
2	B	340	ILE	N-CA-C	-5.64	105.01	110.42
1	A	133	ALA	N-CA-C	5.64	118.15	111.33
1	A	598	PRO	N-CA-CB	5.64	108.34	103.27
1	C	16	PRO	N-CA-CB	5.64	108.58	103.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIS	CB-CG-ND1	5.63	131.15	122.70
2	B	617	LEU	N-CA-C	-5.63	99.23	108.41
2	D	370	PRO	N-CA-CB	5.63	108.32	103.31
1	A	88	GLN	CA-C-N	5.63	128.83	120.95
1	A	88	GLN	C-N-CA	5.63	128.83	120.95
2	D	273	ALA	CA-C-N	5.63	127.82	120.28
2	D	273	ALA	C-N-CA	5.63	127.82	120.28
1	C	423	HIS	CA-CB-CG	5.63	119.43	113.80
2	D	465	GLU	CA-C-O	5.63	126.56	120.32
2	B	311	PHE	CA-CB-CG	5.62	119.42	113.80
2	D	528	GLU	O-C-N	-5.62	115.75	122.15
1	A	337	THR	CA-C-O	5.62	128.35	121.56
1	C	120	PRO	CA-C-N	5.62	127.74	120.44
1	C	120	PRO	C-N-CA	5.62	127.74	120.44
1	C	675	LEU	O-C-N	-5.62	115.15	122.39
2	B	345	ILE	CA-C-N	5.61	128.26	120.29
2	B	345	ILE	C-N-CA	5.61	128.26	120.29
2	B	128	GLY	CA-C-O	-5.61	114.97	120.75
2	B	528	GLU	O-C-N	-5.61	115.75	122.15
1	A	394	SER	O-C-N	-5.61	115.66	122.22
1	A	104	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	368	LEU	N-CA-C	5.61	118.93	111.75
2	D	419	GLU	CA-C-O	5.61	126.41	119.79
2	B	184	GLU	O-C-N	-5.61	116.18	122.12
1	C	668	LEU	CA-C-N	5.60	127.72	120.44
1	C	668	LEU	C-N-CA	5.60	127.72	120.44
1	C	69	PRO	CA-C-N	5.60	132.24	121.54
1	C	69	PRO	C-N-CA	5.60	132.24	121.54
2	D	340	ILE	CA-C-N	5.60	128.24	120.29
2	D	340	ILE	C-N-CA	5.60	128.24	120.29
1	A	514	LYS	O-C-N	-5.60	116.31	122.07
1	A	196	ILE	N-CA-C	-5.59	100.28	108.11
1	A	526	ASP	CA-C-O	5.59	125.57	120.09
1	C	380	ALA	O-C-N	-5.59	115.67	122.22
1	C	402	PRO	N-CA-C	5.59	121.20	113.65
1	A	328	HIS	N-CA-C	-5.59	101.17	110.17
1	A	550	ASP	N-CA-C	-5.59	105.27	111.36
1	A	666	PRO	O-C-N	-5.59	115.85	122.17
2	B	60	LYS	O-C-N	-5.59	116.28	122.09
2	B	465	GLU	CA-C-O	5.59	126.53	120.32
1	A	684	VAL	CA-C-O	5.59	126.28	120.36
2	B	165	GLU	CB-CG-CD	5.58	122.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	PRO	O-C-N	-5.58	114.71	122.30
2	D	150	LEU	CA-C-N	5.58	127.76	120.28
2	D	150	LEU	C-N-CA	5.58	127.76	120.28
2	D	204	PHE	CA-C-N	5.58	127.70	120.44
2	D	204	PHE	C-N-CA	5.58	127.70	120.44
2	B	67	VAL	CA-C-N	5.58	131.75	122.66
2	B	67	VAL	C-N-CA	5.58	131.75	122.66
2	B	201	PRO	N-CA-CB	5.58	109.20	103.23
2	B	157	VAL	CB-CA-C	-5.58	105.27	111.35
2	B	283	ARG	N-CA-CB	5.57	119.72	110.47
1	C	80	ALA	N-CA-C	-5.57	105.20	111.28
1	C	447	GLU	CA-C-N	5.57	127.69	120.44
1	C	447	GLU	C-N-CA	5.57	127.69	120.44
1	C	504	ASP	CA-C-N	5.57	125.41	119.28
1	C	504	ASP	C-N-CA	5.57	125.41	119.28
2	B	31	THR	CA-C-N	5.57	127.68	120.44
2	B	31	THR	C-N-CA	5.57	127.68	120.44
2	D	257	ALA	CA-C-N	5.57	127.74	120.28
2	D	257	ALA	C-N-CA	5.57	127.74	120.28
1	A	426	GLU	N-CA-C	-5.57	105.13	111.14
1	C	502	GLU	N-CA-C	5.57	118.28	111.82
2	B	581	VAL	O-C-N	-5.57	116.46	121.91
1	C	443	LYS	O-C-N	-5.57	116.30	122.09
2	B	534	VAL	CA-C-N	5.56	127.74	120.28
2	B	534	VAL	C-N-CA	5.56	127.74	120.28
1	C	674	LYS	O-C-N	-5.56	114.97	122.43
1	C	534	LEU	O-C-N	-5.56	115.43	122.27
1	A	206	VAL	CA-CB-CG1	5.56	119.85	110.40
1	A	150	ARG	CA-C-N	5.56	128.76	120.31
1	A	150	ARG	C-N-CA	5.56	128.76	120.31
1	C	131	ARG	CD-NE-CZ	5.56	132.18	124.40
1	C	206	VAL	CB-CA-C	-5.55	102.18	111.29
1	C	397	THR	O-C-N	-5.55	115.05	122.49
1	A	414	TRP	CA-C-N	5.55	127.66	120.44
1	A	414	TRP	C-N-CA	5.55	127.66	120.44
2	D	24	ALA	CA-C-O	5.55	126.36	119.97
1	C	271	GLU	O-C-N	-5.55	116.35	122.07
1	A	393	GLU	N-CA-CB	-5.55	103.21	110.59
2	B	306	ARG	CA-C-N	5.55	127.55	120.56
2	B	306	ARG	C-N-CA	5.55	127.55	120.56
2	B	380	ARG	CA-C-N	5.55	128.74	120.31
2	B	380	ARG	C-N-CA	5.55	128.74	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	PRO	CA-C-N	5.55	126.77	119.84
1	C	213	PRO	C-N-CA	5.55	126.77	119.84
1	C	376	THR	N-CA-C	-5.55	101.76	110.36
2	D	507	VAL	CA-C-N	5.55	130.11	120.68
2	D	507	VAL	C-N-CA	5.55	130.11	120.68
2	B	115	ASP	CA-C-N	5.54	124.74	118.97
2	B	115	ASP	C-N-CA	5.54	124.74	118.97
1	A	587	VAL	CA-C-N	5.54	127.65	120.44
1	A	587	VAL	C-N-CA	5.54	127.65	120.44
1	C	150	ARG	CA-CB-CG	5.54	125.19	114.10
1	C	494	ALA	O-C-N	-5.54	116.25	122.12
1	A	568	GLY	N-CA-C	5.54	122.73	115.36
2	D	101	ASN	N-CA-C	5.54	119.90	113.20
1	C	104	ARG	CA-C-N	5.54	127.70	120.28
1	C	104	ARG	C-N-CA	5.54	127.70	120.28
1	A	343	ASN	O-C-N	-5.54	115.46	122.27
2	B	169	ARG	CD-NE-CZ	5.54	132.15	124.40
1	A	677	ARG	CA-C-N	5.53	127.59	120.89
1	A	677	ARG	C-N-CA	5.53	127.59	120.89
2	B	369	LEU	CA-C-O	5.53	125.58	120.60
2	D	401	GLY	O-C-N	-5.53	116.01	122.60
1	C	317	PRO	N-CA-CB	5.53	108.48	103.34
1	C	319	ASN	CA-C-N	5.53	125.36	119.28
1	C	319	ASN	C-N-CA	5.53	125.36	119.28
1	C	426	GLU	CA-C-N	5.53	127.53	120.56
1	C	426	GLU	C-N-CA	5.53	127.53	120.56
2	D	66	THR	O-C-N	-5.53	115.90	122.65
1	A	8	ASP	N-CA-C	5.53	119.51	112.87
1	C	252	ALA	CA-C-N	5.53	127.69	120.28
1	C	252	ALA	C-N-CA	5.53	127.69	120.28
1	C	677	ARG	CA-CB-CG	5.53	125.16	114.10
2	D	239	ASN	CA-C-O	5.53	126.18	119.38
1	A	621	TYR	CA-C-O	-5.53	114.56	120.42
2	D	115	ASP	CA-C-N	5.53	124.72	118.97
2	D	115	ASP	C-N-CA	5.53	124.72	118.97
1	C	552	LEU	CA-C-N	5.52	127.68	120.28
1	C	552	LEU	C-N-CA	5.52	127.68	120.28
1	C	395	GLY	O-C-N	-5.52	115.01	122.35
1	C	55	TYR	N-CA-C	5.52	119.11	112.38
1	C	505	PRO	N-CA-CB	5.52	109.35	103.39
1	C	263	GLY	CA-C-N	5.52	127.51	120.56
1	C	263	GLY	C-N-CA	5.52	127.51	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	TRP	CA-C-N	5.51	127.98	120.54
2	B	35	TRP	C-N-CA	5.51	127.98	120.54
1	C	385	ASN	O-C-N	-5.51	115.77	122.22
2	D	201	PRO	N-CA-CB	5.51	109.39	103.33
2	B	310	VAL	CA-C-N	5.51	132.36	122.38
2	B	310	VAL	C-N-CA	5.51	132.36	122.38
1	C	214	PRO	N-CA-CB	5.51	109.04	103.25
1	C	427	VAL	CA-C-N	5.51	128.22	120.28
1	C	427	VAL	C-N-CA	5.51	128.22	120.28
2	B	242	HIS	O-C-N	-5.51	116.39	122.07
2	B	461	THR	CA-CB-OG1	-5.51	101.34	109.60
2	D	276	ALA	CA-C-N	5.51	127.60	120.44
2	D	276	ALA	C-N-CA	5.51	127.60	120.44
1	A	538	ALA	CA-C-N	5.51	126.06	120.00
1	A	538	ALA	C-N-CA	5.51	126.06	120.00
2	B	190	ALA	CA-C-N	5.50	131.23	120.99
2	B	190	ALA	C-N-CA	5.50	131.23	120.99
1	C	529	ARG	N-CA-CB	-5.50	102.33	110.53
2	B	501	MET	CA-C-N	5.50	127.65	120.28
2	B	501	MET	C-N-CA	5.50	127.65	120.28
2	B	556	ALA	CA-C-N	5.50	127.59	120.44
2	B	556	ALA	C-N-CA	5.50	127.59	120.44
1	C	550	ASP	N-CA-C	-5.50	105.36	111.36
1	A	24	ARG	CG-CD-NE	5.50	124.11	112.00
2	B	149	HIS	CA-C-N	5.50	127.97	120.54
2	B	149	HIS	C-N-CA	5.50	127.97	120.54
2	B	602	PHE	CA-C-N	5.50	129.55	120.25
2	B	602	PHE	C-N-CA	5.50	129.55	120.25
2	B	417	TRP	CA-C-N	5.50	127.65	120.28
2	B	417	TRP	C-N-CA	5.50	127.65	120.28
1	A	712	PRO	O-C-N	-5.49	115.92	122.24
2	B	230	ASP	CA-C-N	5.49	128.67	120.87
2	B	230	ASP	C-N-CA	5.49	128.67	120.87
2	D	584	ALA	CA-C-N	5.49	127.58	120.44
2	D	584	ALA	C-N-CA	5.49	127.58	120.44
2	B	205	ALA	CA-C-N	5.49	127.64	120.28
2	B	205	ALA	C-N-CA	5.49	127.64	120.28
2	D	417	TRP	CA-C-N	5.49	128.19	120.28
2	D	417	TRP	C-N-CA	5.49	128.19	120.28
1	A	375	PRO	N-CA-CB	5.49	108.12	103.35
1	A	141	VAL	N-CA-C	5.48	116.16	109.30
1	A	377	ASP	CA-C-N	5.48	127.89	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ASP	C-N-CA	5.48	127.89	120.65
2	D	466	PHE	CA-C-O	5.48	124.65	120.26
1	A	435	LYS	O-C-N	-5.48	116.31	122.12
2	B	410	ARG	CA-C-N	5.48	127.56	120.44
2	B	410	ARG	C-N-CA	5.48	127.56	120.44
2	B	268	GLU	N-CA-C	-5.48	105.00	110.97
1	C	622	ALA	CA-C-N	5.48	129.36	120.60
1	C	622	ALA	C-N-CA	5.48	129.36	120.60
2	B	415	ALA	O-C-N	-5.47	115.91	122.15
1	C	357	GLN	CA-C-O	5.47	126.11	119.11
2	D	510	ARG	CA-C-O	5.47	124.89	119.75
1	A	488	VAL	CB-CA-C	-5.47	104.86	112.02
1	A	513	ASP	O-C-N	-5.47	116.32	122.12
2	D	602	PHE	CA-C-N	5.47	129.49	120.25
2	D	602	PHE	C-N-CA	5.47	129.49	120.25
2	B	419	GLU	O-C-N	-5.47	115.92	122.15
2	D	104	MET	CA-C-O	-5.47	114.76	120.55
1	C	64	TYR	CA-CB-CG	-5.46	104.07	113.90
1	A	321	LYS	O-C-N	-5.46	115.83	122.22
1	C	285	SER	O-C-N	-5.46	116.05	123.15
1	C	286	PHE	CA-CB-CG	-5.46	108.34	113.80
1	C	382	ILE	N-CA-C	-5.46	105.40	110.53
1	A	486	SER	CA-C-O	-5.46	114.77	120.55
1	C	617	ILE	CA-C-N	5.46	128.37	120.79
1	C	617	ILE	C-N-CA	5.46	128.37	120.79
1	A	176	ALA	CB-CA-C	-5.45	102.32	110.88
2	B	89	GLY	O-C-N	-5.45	115.47	122.39
1	A	168	ASN	OD1-CG-ND2	-5.45	117.15	122.60
2	B	273	ALA	N-CA-C	-5.45	104.98	111.69
1	C	179	VAL	O-C-N	-5.45	116.57	121.91
2	B	189	PRO	N-CA-CB	5.45	108.97	103.25
2	D	171	ASP	CA-C-N	5.45	127.52	120.44
2	D	171	ASP	C-N-CA	5.45	127.52	120.44
2	D	455	ASN	O-C-N	-5.45	115.53	122.34
2	D	362	PRO	N-CA-CB	5.45	108.51	103.39
1	C	79	TYR	N-CA-C	5.44	119.18	112.54
1	C	357	GLN	O-C-N	-5.44	114.48	122.43
1	C	621	TYR	CA-C-N	5.44	128.02	120.29
1	C	621	TYR	C-N-CA	5.44	128.02	120.29
1	C	115	VAL	N-CA-C	5.44	116.55	108.23
1	A	528	ASP	O-C-N	-5.44	115.32	122.39
1	C	281	ALA	N-CA-CB	5.44	118.40	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	ASP	CA-C-O	5.43	126.57	120.92
1	C	208	ASN	N-CA-C	5.43	118.93	111.54
2	B	363	PHE	O-C-N	-5.43	115.87	122.22
1	A	53	ASP	CA-C-N	5.42	129.04	120.47
1	A	53	ASP	C-N-CA	5.42	129.04	120.47
1	A	524	ASP	CA-CB-CG	5.42	118.03	112.60
1	A	319	ASN	CA-C-O	5.42	125.39	119.32
1	C	414	TRP	CA-C-N	5.42	127.49	120.44
1	C	414	TRP	C-N-CA	5.42	127.49	120.44
1	A	589	GLU	CA-C-N	5.42	127.49	120.44
1	A	589	GLU	C-N-CA	5.42	127.49	120.44
2	B	510	ARG	CA-C-N	5.42	125.36	119.78
2	B	510	ARG	C-N-CA	5.42	125.36	119.78
1	A	89	TYR	CA-CB-CG	5.42	123.66	113.90
1	A	276	ASN	O-C-N	-5.42	116.61	122.79
2	B	85	LEU	CA-C-N	-5.42	114.21	122.06
2	B	85	LEU	C-N-CA	-5.42	114.21	122.06
2	D	290	GLN	N-CA-C	5.42	117.63	111.02
1	C	281	ALA	CA-C-N	5.42	125.08	119.56
1	C	281	ALA	C-N-CA	5.42	125.08	119.56
1	A	204	PHE	CA-CB-CG	-5.41	108.39	113.80
2	B	200	ASP	CA-C-O	5.41	127.58	120.16
2	B	532	SER	CA-C-N	5.41	125.49	119.32
2	B	532	SER	C-N-CA	5.41	125.49	119.32
1	C	14	ASN	CA-CB-CG	5.41	118.01	112.60
1	C	351	GLU	O-C-N	-5.41	115.98	122.15
1	C	697	ARG	CD-NE-CZ	5.41	131.98	124.40
1	A	504	ASP	CA-CB-CG	5.41	118.01	112.60
2	B	233	ALA	CA-C-O	5.41	126.60	120.00
1	A	327	THR	CA-C-O	5.41	127.77	121.44
1	A	61	LEU	N-CA-C	5.41	118.98	112.38
1	C	445	ARG	O-C-N	-5.41	116.39	122.12
2	B	243	ASN	CA-C-O	5.40	126.21	120.10
1	C	8	ASP	N-CA-C	5.40	119.62	113.19
1	C	94	THR	CA-C-O	5.40	128.25	121.66
1	C	651	VAL	N-CA-C	5.40	116.45	108.45
1	A	524	ASP	O-C-N	-5.40	115.37	122.39
1	C	121	THR	O-C-N	-5.40	116.51	122.07
1	C	486	SER	CA-C-O	-5.40	114.83	120.55
2	D	571	ALA	CA-C-N	5.39	128.51	120.31
2	D	571	ALA	C-N-CA	5.39	128.51	120.31
1	A	298	VAL	N-CA-C	-5.39	105.25	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	SER	O-C-N	-5.39	116.00	122.15
1	C	622	ALA	O-C-N	-5.39	116.00	122.15
2	B	49	PRO	CA-C-N	5.39	131.43	122.54
2	B	49	PRO	C-N-CA	5.39	131.43	122.54
2	B	265	ALA	CA-C-N	5.39	128.04	120.28
2	B	265	ALA	C-N-CA	5.39	128.04	120.28
1	C	518	ALA	O-C-N	-5.39	116.41	122.12
1	A	177	LEU	CA-C-N	5.38	127.76	120.44
1	A	177	LEU	C-N-CA	5.38	127.76	120.44
2	B	69	GLY	CA-C-N	-5.38	115.42	122.37
2	B	69	GLY	C-N-CA	-5.38	115.42	122.37
2	D	88	PRO	N-CA-CB	5.38	108.30	103.19
2	D	229	PRO	CA-C-O	5.38	125.55	118.98
2	D	374	PHE	CA-C-N	5.38	125.02	119.05
2	D	374	PHE	C-N-CA	5.38	125.02	119.05
1	C	262	ASP	CA-C-N	5.38	125.95	119.98
1	C	262	ASP	C-N-CA	5.38	125.95	119.98
1	A	198	ASN	N-CA-CB	-5.38	101.40	110.49
1	A	553	GLU	O-C-N	-5.38	115.65	122.27
1	A	674	LYS	CA-CB-CG	5.37	124.85	114.10
2	D	407	SER	CA-C-N	5.37	129.81	120.68
2	D	407	SER	C-N-CA	5.37	129.81	120.68
1	C	676	GLY	O-C-N	-5.37	116.04	122.33
1	A	170	ALA	O-C-N	-5.37	112.94	121.53
2	B	276	ALA	N-CA-C	-5.37	105.34	111.14
1	C	623	ASP	CA-CB-CG	5.37	117.97	112.60
2	D	494	SER	CA-C-N	5.37	127.73	120.38
2	D	494	SER	C-N-CA	5.37	127.73	120.38
2	D	534	VAL	O-C-N	-5.37	116.65	121.91
1	A	621	TYR	CA-C-N	5.37	127.47	120.28
1	A	621	TYR	C-N-CA	5.37	127.47	120.28
2	B	466	PHE	CA-C-O	5.37	124.55	120.26
1	C	236	ASN	N-CA-C	-5.37	101.04	109.25
1	C	241	SER	CB-CA-C	-5.36	99.56	109.37
1	C	320	PRO	N-CA-CB	5.36	109.18	103.39
1	A	237	SER	CA-C-O	5.36	125.97	119.11
2	B	115	ASP	CA-C-O	5.36	123.59	119.46
1	A	281	ALA	CA-C-N	5.36	125.03	119.56
1	A	281	ALA	C-N-CA	5.36	125.03	119.56
2	B	288	HIS	CB-CG-CD2	5.36	138.16	131.20
2	B	235	THR	N-CA-CB	5.36	120.22	110.95
2	B	407	SER	CA-C-N	5.35	127.99	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	407	SER	C-N-CA	5.35	127.99	120.28
1	A	619	THR	O-C-N	-5.35	116.56	122.07
1	C	411	GLU	CA-C-N	5.35	127.45	120.28
1	C	411	GLU	C-N-CA	5.35	127.45	120.28
1	A	505	PRO	N-CA-CB	5.35	108.64	103.51
1	C	578	PRO	N-CA-CB	5.35	109.19	103.52
2	B	531	SER	N-CA-C	5.34	116.91	111.14
1	C	698	LYS	CA-C-N	5.34	132.00	121.58
1	C	698	LYS	C-N-CA	5.34	132.00	121.58
2	B	24	ALA	O-C-N	-5.34	115.70	122.27
2	D	455	ASN	N-CA-CB	5.34	118.39	110.49
1	A	191	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	576	ASN	N-CA-C	5.34	120.98	113.56
1	A	393	GLU	N-CA-C	5.33	120.44	113.88
1	C	579	GLU	N-CA-C	-5.33	105.13	111.69
1	A	689	PRO	N-CA-CB	5.33	108.06	103.31
1	A	540	ARG	O-C-N	-5.33	116.07	122.15
2	D	348	PHE	CA-C-N	5.33	127.42	120.28
2	D	348	PHE	C-N-CA	5.33	127.42	120.28
2	D	601	GLU	CA-C-O	5.33	125.81	119.10
2	D	189	PRO	N-CA-CB	5.33	108.84	103.25
2	B	333	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	D	315	GLU	CA-C-N	5.32	129.61	120.72
2	D	315	GLU	C-N-CA	5.32	129.61	120.72
2	B	257	ALA	O-C-N	-5.32	116.59	122.07
2	B	110	ARG	CD-NE-CZ	5.32	131.85	124.40
1	C	345	VAL	CA-C-N	5.32	127.37	120.56
1	C	345	VAL	C-N-CA	5.32	127.37	120.56
1	C	595	GLY	CA-C-O	5.32	125.18	119.06
2	D	375	PRO	N-CA-CB	5.32	109.18	103.33
1	A	284	LEU	N-CA-C	-5.32	101.80	110.20
1	A	218	MET	O-C-N	-5.31	116.49	122.12
2	D	452	ARG	CA-C-N	5.31	127.67	120.44
2	D	452	ARG	C-N-CA	5.31	127.67	120.44
2	B	490	TRP	CA-C-N	5.31	130.26	122.77
2	B	490	TRP	C-N-CA	5.31	130.26	122.77
2	D	554	VAL	O-C-N	-5.31	116.72	121.87
1	A	56	LYS	O-C-N	-5.31	115.53	122.59
2	B	386	LEU	O-C-N	-5.31	116.49	122.12
1	C	368	LEU	N-CA-C	5.31	117.81	111.71
2	D	477	LYS	N-CA-CB	5.31	118.17	110.32
1	A	699	ASP	CA-CB-CG	5.31	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	256	LEU	O-C-N	-5.30	116.61	122.07
1	A	52	GLU	N-CA-C	5.30	118.84	112.38
1	C	528	ASP	O-C-N	-5.30	115.38	122.43
2	D	75	MET	O-C-N	-5.30	116.81	123.27
1	A	493	LYS	CA-C-N	5.29	127.38	120.28
1	A	493	LYS	C-N-CA	5.29	127.38	120.28
1	C	463	PRO	N-CA-CB	5.29	108.02	103.31
1	A	79	TYR	N-CA-C	5.29	119.00	112.54
1	A	590	PHE	CA-C-O	-5.29	115.26	120.82
1	C	430	VAL	N-CA-CB	-5.29	102.50	111.23
1	A	138	MET	N-CA-C	5.29	118.89	112.23
2	B	441	VAL	CA-C-N	5.29	127.37	120.28
2	B	441	VAL	C-N-CA	5.29	127.37	120.28
1	A	683	THR	N-CA-C	-5.29	101.26	109.72
1	C	383	ALA	O-C-N	-5.28	116.63	122.07
2	B	269	GLN	N-CA-C	5.28	122.04	110.80
2	B	465	GLU	O-C-N	-5.28	117.14	123.31
2	D	205	ALA	N-CA-C	-5.28	105.42	111.07
1	A	368	LEU	O-C-N	-5.28	116.19	122.20
2	D	501	MET	CA-C-N	5.28	127.35	120.28
2	D	501	MET	C-N-CA	5.28	127.35	120.28
1	A	672	LEU	CA-C-N	5.27	127.61	120.65
1	A	672	LEU	C-N-CA	5.27	127.61	120.65
2	B	383	GLY	CA-C-N	5.27	127.69	120.46
2	B	383	GLY	C-N-CA	5.27	127.69	120.46
1	A	646	GLU	O-C-N	-5.27	116.05	122.22
1	C	495	LYS	CA-C-N	5.27	127.78	120.29
1	C	495	LYS	C-N-CA	5.27	127.78	120.29
2	D	202	ILE	O-C-N	-5.27	116.42	121.90
1	A	315	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	94	THR	O-C-N	-5.27	117.04	122.94
1	C	7	PHE	N-CA-C	5.27	119.58	113.20
1	A	66	GLY	CA-C-N	5.27	131.88	122.13
1	A	66	GLY	C-N-CA	5.27	131.88	122.13
1	A	698	LYS	CA-C-N	5.27	131.85	121.58
1	A	698	LYS	C-N-CA	5.27	131.85	121.58
2	B	376	LEU	CA-C-N	5.27	127.34	120.28
2	B	376	LEU	C-N-CA	5.27	127.34	120.28
2	B	435	THR	CA-C-N	5.27	131.86	122.06
2	B	435	THR	C-N-CA	5.27	131.86	122.06
2	D	599	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	455	ALA	O-C-N	-5.27	116.65	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	345	ILE	CA-C-N	5.27	127.28	120.44
2	D	345	ILE	C-N-CA	5.27	127.28	120.44
1	C	509	LYS	CA-C-N	5.26	127.60	120.65
1	C	509	LYS	C-N-CA	5.26	127.60	120.65
2	D	384	ILE	O-C-N	-5.26	116.77	121.87
1	C	310	LYS	O-C-N	-5.26	116.45	122.08
2	D	107	TRP	N-CA-C	-5.26	102.41	110.14
2	B	251	GLU	CB-CG-CD	5.26	121.53	112.60
2	B	348	PHE	CB-CA-C	-5.26	102.63	110.88
1	C	445	ARG	CA-C-N	5.26	127.88	120.42
1	C	445	ARG	C-N-CA	5.26	127.88	120.42
2	D	628	SER	CA-C-N	5.26	127.27	120.44
2	D	628	SER	C-N-CA	5.26	127.27	120.44
1	A	623	ASP	O-C-N	-5.25	115.39	122.43
2	D	36	GLU	O-C-N	-5.25	116.55	122.12
1	A	28	LEU	CA-C-N	5.25	127.31	120.28
1	A	28	LEU	C-N-CA	5.25	127.31	120.28
1	C	404	SER	CA-C-O	5.25	125.81	120.88
2	D	240	ILE	N-CA-C	-5.25	105.38	110.42
1	C	344	ASN	CA-C-N	5.25	127.65	120.46
1	C	344	ASN	C-N-CA	5.25	127.65	120.46
1	C	671	GLU	CA-C-N	5.24	127.26	120.44
1	C	671	GLU	C-N-CA	5.24	127.26	120.44
2	D	331	LEU	CA-C-O	5.24	127.03	121.16
2	B	114	GLU	CA-CB-CG	5.24	124.57	114.10
2	B	61	ARG	O-C-N	-5.23	116.10	122.22
2	B	363	PHE	N-CA-C	5.23	117.73	111.71
1	C	268	ARG	O-C-N	-5.23	116.65	122.09
2	D	586	LYS	O-C-N	-5.23	116.58	122.12
2	B	238	ALA	O-C-N	-5.23	115.84	122.27
2	D	104	MET	N-CA-C	5.23	116.98	111.28
1	A	513	ASP	CA-C-N	5.23	127.23	120.44
1	A	513	ASP	C-N-CA	5.23	127.23	120.44
1	A	311	LEU	O-C-N	-5.22	116.69	122.07
1	A	496	LEU	CA-C-N	5.22	127.24	120.56
1	A	496	LEU	C-N-CA	5.22	127.24	120.56
1	A	707	PRO	N-CA-CB	5.22	107.84	103.25
2	B	44	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	434	ALA	O-C-N	-5.22	116.70	122.07
1	A	317	PRO	N-CA-CB	5.21	108.19	103.34
2	B	258	THR	CA-C-N	5.21	125.62	119.94
2	B	258	THR	C-N-CA	5.21	125.62	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	392	GLN	N-CA-C	5.21	119.69	112.45
1	A	128	ASP	N-CA-CB	5.21	118.32	110.30
1	C	43	GLN	CA-C-O	5.21	127.60	121.40
2	B	266	LEU	CA-C-N	5.21	127.82	120.42
2	B	266	LEU	C-N-CA	5.21	127.82	120.42
1	A	182	ALA	N-CA-C	-5.20	105.30	110.97
1	A	433	MET	CB-CG-SD	5.20	128.31	112.70
1	C	268	ARG	NE-CZ-NH2	-5.20	114.52	119.20
2	D	537	ILE	O-C-N	-5.20	116.74	121.94
2	B	276	ALA	CA-C-N	5.20	127.25	120.28
2	B	276	ALA	C-N-CA	5.20	127.25	120.28
1	C	661	HIS	N-CA-C	5.20	117.69	111.71
2	D	147	PRO	N-CA-CB	5.20	109.00	103.39
1	A	466	GLY	CA-C-N	5.19	131.32	121.97
1	A	466	GLY	C-N-CA	5.19	131.32	121.97
1	A	266	TYR	O-C-N	-5.19	116.14	122.22
1	A	535	CYS	O-C-N	-5.19	115.37	122.33
2	B	298	ARG	CA-C-N	5.19	127.24	120.28
2	B	298	ARG	C-N-CA	5.19	127.24	120.28
2	D	575	ALA	N-CA-C	-5.19	105.32	110.97
1	C	163	VAL	CA-C-O	5.19	125.78	120.39
1	C	218	MET	O-C-N	-5.18	116.62	122.12
2	D	382	THR	N-CA-C	-5.18	104.70	111.02
2	B	104	MET	CA-C-O	-5.18	115.06	120.55
2	B	159	LEU	CA-C-N	5.18	129.49	120.68
2	B	159	LEU	C-N-CA	5.18	129.49	120.68
1	C	425	GLN	CB-CG-CD	-5.18	103.80	112.60
1	A	529	ARG	N-CA-CB	-5.18	102.82	110.53
2	B	274	THR	CA-C-N	5.18	128.18	120.31
2	B	274	THR	C-N-CA	5.18	128.18	120.31
2	B	543	PRO	N-CA-CB	5.17	108.14	103.33
1	C	610	HIS	CA-C-N	-5.17	113.22	121.44
1	C	610	HIS	C-N-CA	-5.17	113.22	121.44
1	C	42	GLU	CA-C-N	5.17	129.96	122.36
1	C	42	GLU	C-N-CA	5.17	129.96	122.36
1	C	635	GLN	CB-CA-C	-5.17	100.80	109.53
2	D	187	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	158	LEU	N-CA-C	5.17	119.21	113.01
1	C	140	GLY	CA-C-O	5.17	126.80	121.38
1	A	276	ASN	N-CA-C	-5.16	103.72	110.53
1	A	314	GLN	O-C-N	-5.16	115.68	122.39
1	A	219	ARG	CA-C-N	5.16	127.06	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	C-N-CA	5.16	127.06	120.56
1	A	225	PHE	CA-C-N	5.16	127.15	120.44
1	A	225	PHE	C-N-CA	5.16	127.15	120.44
2	B	55	PHE	N-CA-CB	5.16	117.49	110.01
2	D	485	ARG	CD-NE-CZ	5.16	131.62	124.40
2	B	510	ARG	CA-C-O	5.16	124.04	119.71
1	C	328	HIS	N-CA-C	-5.16	101.87	110.17
1	A	172	LEU	CA-C-N	5.16	124.66	119.19
1	A	172	LEU	C-N-CA	5.16	124.66	119.19
1	C	695	GLU	CA-C-N	5.16	127.14	120.44
1	C	695	GLU	C-N-CA	5.16	127.14	120.44
1	A	369	ASP	CA-C-O	5.15	125.93	119.59
1	A	335	SER	CA-C-N	5.15	129.71	122.09
1	A	335	SER	C-N-CA	5.15	129.71	122.09
1	C	127	SER	N-CA-C	5.15	118.82	112.54
1	C	545	VAL	CA-C-N	5.15	125.66	119.94
1	C	545	VAL	C-N-CA	5.15	125.66	119.94
1	A	64	TYR	N-CA-C	5.15	117.79	109.40
1	A	319	ASN	OD1-CG-ND2	-5.15	117.45	122.60
2	D	524	PHE	CA-CB-CG	5.15	118.95	113.80
2	B	524	PHE	CA-CB-CG	5.15	118.95	113.80
2	B	275	GLU	CA-C-N	5.14	127.44	120.44
2	B	275	GLU	C-N-CA	5.14	127.44	120.44
2	B	523	ASP	N-CA-C	5.14	116.69	111.14
1	C	379	SER	CA-C-N	5.14	127.68	120.28
1	C	379	SER	C-N-CA	5.14	127.68	120.28
1	A	180	VAL	CB-CA-C	5.14	118.55	111.97
1	C	95	ALA	CA-C-N	5.14	127.12	120.44
1	C	95	ALA	C-N-CA	5.14	127.12	120.44
1	C	217	SER	N-CA-C	-5.14	105.57	111.07
2	B	77	ARG	CA-C-O	5.14	127.20	120.16
1	C	660	GLY	CA-C-N	5.14	127.67	120.28
1	C	660	GLY	C-N-CA	5.14	127.67	120.28
2	D	35	TRP	CA-C-N	5.14	127.16	120.28
2	D	35	TRP	C-N-CA	5.14	127.16	120.28
2	D	78	PRO	N-CA-CB	5.14	109.11	103.26
2	D	498	GLU	CA-C-N	5.14	128.12	120.31
2	D	498	GLU	C-N-CA	5.14	128.12	120.31
1	A	671	GLU	CA-C-N	5.13	127.42	120.44
1	A	671	GLU	C-N-CA	5.13	127.42	120.44
2	B	599	PHE	O-C-N	-5.13	115.55	122.43
1	C	67	ILE	CA-CB-CG1	5.13	119.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	SER	O-C-N	-5.13	116.22	122.22
1	A	541	ALA	O-C-N	-5.13	114.80	122.39
1	A	633	LEU	N-CA-C	-5.13	104.10	110.41
2	D	419	GLU	CB-CG-CD	5.13	121.31	112.60
2	B	215	THR	N-CA-C	5.12	118.79	112.54
2	D	86	GLY	N-CA-C	-5.12	105.22	112.81
2	D	157	VAL	N-CA-C	5.12	114.99	108.12
2	B	398	PRO	N-CA-CB	5.12	108.92	103.39
1	C	469	LYS	CA-C-O	5.12	126.39	120.14
1	A	67	ILE	CA-CB-CG1	5.12	119.11	110.40
1	A	189	PRO	N-CA-CB	5.12	109.10	103.26
1	A	264	VAL	O-C-N	-5.12	116.90	121.87
1	C	465	ILE	N-CA-C	5.12	116.28	109.37
2	D	490	TRP	CA-C-N	5.12	129.99	122.77
2	D	490	TRP	C-N-CA	5.12	129.99	122.77
1	C	475	GLU	CA-C-N	5.12	123.40	119.66
1	C	475	GLU	C-N-CA	5.12	123.40	119.66
1	C	192	LEU	N-CA-C	5.12	116.65	108.41
1	A	377	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	462	ALA	CA-C-N	5.11	131.17	121.97
2	B	462	ALA	C-N-CA	5.11	131.17	121.97
1	C	27	GLU	CA-C-N	5.11	127.09	120.44
1	C	27	GLU	C-N-CA	5.11	127.09	120.44
1	A	341	VAL	CA-C-O	-5.11	115.10	120.57
1	A	180	VAL	O-C-N	-5.11	116.90	121.91
1	C	103	ARG	CD-NE-CZ	5.11	131.55	124.40
1	C	714	SER	CA-C-N	5.11	127.39	120.44
1	C	714	SER	C-N-CA	5.11	127.39	120.44
1	A	682	ILE	N-CA-CB	5.11	118.97	111.52
1	A	48	THR	N-CA-C	5.10	119.50	113.28
2	D	268	GLU	O-C-N	-5.10	116.73	122.03
1	A	252	ALA	N-CA-C	5.10	117.23	111.11
1	A	292	MET	O-C-N	-5.10	115.60	122.43
1	C	524	ASP	O-C-N	-5.10	115.77	122.39
2	D	265	ALA	CA-C-N	5.10	127.11	120.28
2	D	265	ALA	C-N-CA	5.10	127.11	120.28
1	A	222	SER	O-C-N	-5.09	116.26	122.22
2	B	292	LEU	CA-C-N	5.09	127.06	120.44
2	B	292	LEU	C-N-CA	5.09	127.06	120.44
2	B	60	LYS	CB-CA-C	-5.09	102.67	110.81
2	B	471	ALA	CA-C-O	-5.09	115.12	120.92
1	C	158	LEU	N-CA-C	5.09	119.12	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	662	LEU	CA-C-O	-5.09	114.12	119.97
1	A	357	GLN	CA-C-N	5.09	133.14	121.34
1	A	357	GLN	C-N-CA	5.09	133.14	121.34
2	B	23	LEU	CA-C-O	5.09	125.00	119.40
1	C	707	PRO	CA-C-O	5.09	127.11	121.36
1	A	350	ILE	O-C-N	-5.08	116.59	121.83
1	C	334	TRP	CA-C-N	5.08	129.21	120.72
1	C	334	TRP	C-N-CA	5.08	129.21	120.72
2	D	348	PHE	CA-CB-CG	5.08	118.88	113.80
2	D	305	ALA	CA-C-N	5.08	127.50	120.29
2	D	305	ALA	C-N-CA	5.08	127.50	120.29
2	B	551	ALA	N-CA-C	-5.08	105.64	111.07
1	C	315	PHE	CA-C-N	5.08	129.84	121.87
1	C	315	PHE	C-N-CA	5.08	129.84	121.87
1	A	198	ASN	O-C-N	-5.08	115.84	122.59
1	A	475	GLU	CA-C-N	5.08	123.36	119.66
1	A	475	GLU	C-N-CA	5.08	123.36	119.66
1	A	645	VAL	CB-CA-C	5.08	118.38	111.88
1	C	178	TYR	N-CA-C	-5.08	105.66	111.14
1	C	243	TYR	O-C-N	-5.08	116.81	122.09
1	C	585	GLU	O-C-N	-5.07	116.81	122.09
2	D	493	ASP	O-C-N	-5.07	116.74	122.12
2	B	322	GLN	CG-CD-NE2	5.07	124.01	116.40
1	C	712	PRO	CA-C-N	5.07	127.08	120.28
1	C	712	PRO	C-N-CA	5.07	127.08	120.28
2	B	262	TYR	N-CA-C	5.07	117.70	111.82
1	C	622	ALA	N-CA-C	-5.07	105.83	111.36
2	B	632	ASP	CA-C-N	5.07	127.67	120.53
2	B	632	ASP	C-N-CA	5.07	127.67	120.53
2	D	42	VAL	O-C-N	-5.07	116.95	121.87
1	A	412	LEU	O-C-N	-5.06	116.75	122.12
1	C	211	ILE	N-CA-CB	5.06	119.58	111.23
1	C	634	PHE	N-CA-C	5.06	119.04	112.86
2	D	218	GLY	O-C-N	-5.06	117.33	122.19
2	D	534	VAL	CA-C-N	5.06	127.07	120.28
2	D	534	VAL	C-N-CA	5.06	127.07	120.28
1	A	208	ASN	N-CA-C	5.06	118.57	111.74
1	A	539	GLY	O-C-N	-5.06	117.28	122.19
1	C	7	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	518	ALA	O-C-N	-5.06	116.76	122.12
2	B	25	GLY	CA-C-O	5.06	125.62	119.65
1	A	8	ASP	O-C-N	-5.06	115.71	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	522	ARG	O-C-N	-5.06	116.76	122.12
1	A	548	MET	CA-C-O	-5.05	115.17	120.63
1	A	251	THR	N-CA-C	-5.05	104.01	110.53
2	B	213	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	379	SER	CA-C-N	5.05	127.55	120.28
1	A	379	SER	C-N-CA	5.05	127.55	120.28
2	B	27	PHE	CA-C-O	5.05	125.86	120.66
2	B	322	GLN	CA-C-O	5.05	125.88	120.38
2	D	75	MET	CA-C-O	5.05	126.47	120.66
2	D	239	ASN	O-C-N	-5.05	115.66	122.43
2	B	56	ALA	O-C-N	-5.04	116.77	122.12
1	C	282	PRO	N-CA-CB	5.04	108.52	103.48
2	D	435	THR	CA-C-N	5.04	130.86	122.54
2	D	435	THR	C-N-CA	5.04	130.86	122.54
1	A	244	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	A	397	THR	O-C-N	-5.04	115.20	122.36
1	C	525	LYS	CA-C-N	5.04	129.87	122.66
1	C	525	LYS	C-N-CA	5.04	129.87	122.66
1	A	403	TRP	CA-C-N	5.04	129.42	121.56
1	A	403	TRP	C-N-CA	5.04	129.42	121.56
1	C	603	ALA	N-CA-C	5.04	118.28	110.17
1	A	251	THR	O-C-N	-5.04	116.46	122.65
2	D	304	TRP	CA-C-N	5.04	127.28	120.38
2	D	304	TRP	C-N-CA	5.04	127.28	120.38
2	D	416	ALA	CA-C-N	5.04	126.99	120.44
2	D	416	ALA	C-N-CA	5.04	126.99	120.44
1	A	290	ILE	N-CA-CB	5.03	118.34	112.35
2	B	260	ALA	CA-C-N	5.03	126.98	120.44
2	B	260	ALA	C-N-CA	5.03	126.98	120.44
1	C	697	ARG	O-C-N	-5.03	116.79	122.12
1	A	130	PRO	N-CA-CB	5.03	108.86	103.33
1	A	294	PHE	N-CA-C	5.03	119.62	111.37
2	B	522	ARG	CA-C-N	5.03	127.28	120.44
2	B	522	ARG	C-N-CA	5.03	127.28	120.44
1	A	134	GLY	CA-C-N	5.03	130.61	121.92
1	A	134	GLY	C-N-CA	5.03	130.61	121.92
1	A	220	ILE	O-C-N	-5.03	116.98	121.91
1	C	304	ALA	O-C-N	-5.03	116.79	122.12
1	C	105	ASN	CA-C-N	5.02	126.97	120.44
1	C	105	ASN	C-N-CA	5.02	126.97	120.44
2	D	283	ARG	N-CA-C	-5.02	99.61	108.20
1	C	527	PRO	CA-C-N	5.02	130.33	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	527	PRO	C-N-CA	5.02	130.33	120.99
2	D	114	GLU	CA-CB-CG	5.02	124.14	114.10
1	C	19	ALA	O-C-N	-5.02	115.70	122.43
1	C	118	ASP	CA-C-N	5.02	126.99	120.26
1	C	118	ASP	C-N-CA	5.02	126.99	120.26
1	C	558	ARG	CD-NE-CZ	5.02	131.42	124.40
1	C	573	GLU	CA-C-O	-5.02	115.55	121.07
2	B	191	LYS	N-CA-C	5.01	118.89	112.87
2	D	588	ALA	N-CA-C	5.01	119.15	113.19
1	A	27	GLU	O-C-N	-5.01	116.81	122.12
2	B	304	TRP	CA-C-N	5.00	126.98	120.28
2	B	304	TRP	C-N-CA	5.00	126.98	120.28
2	D	458	GLN	N-CA-CB	5.00	118.57	111.21
2	D	559	LYS	O-C-N	-5.00	116.82	122.12
2	D	413	ALA	CA-C-N	5.00	127.48	120.28
2	D	413	ALA	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5575	0	5482	42	0
1	C	5575	0	5482	40	0
2	B	4718	0	4672	41	0
2	D	4718	0	4672	41	0
3	A	91	0	88	17	0
3	C	91	0	88	11	0
4	A	55	0	35	2	0
4	C	55	0	35	5	0
5	A	55	0	35	1	0
5	C	55	0	35	1	0
6	A	18	0	13	1	0
6	C	18	0	13	1	0
7	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	D	6	0	8	0	0
8	A	404	0	0	0	0
8	B	239	0	0	1	0
8	C	400	0	0	2	0
8	D	243	0	0	1	0
All	All	22334	0	20682	188	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 (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:800:B12:H531	3:C:800:B12:H552	1.35	1.09
3:A:800:B12:H552	3:A:800:B12:H531	1.31	1.07
4:C:801[A]:SCA:H92	4:C:801[A]:SCA:NP2	1.88	0.85
1:A:638:GLU:HA	1:A:671:GLU:HG2	1.60	0.81
3:A:800:B12:H531	3:A:800:B12:C55	2.07	0.81
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.63	0.80
2:B:468:MET:HE2	2:B:471:ALA:HA	1.64	0.79
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.66	0.76
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.66	0.76
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.68	0.76
3:C:800:B12:H531	3:C:800:B12:C55	2.08	0.74
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.70	0.73
1:A:650:HIS:HB3	1:A:722:LEU:HD11	1.68	0.73
2:D:237:ASP:HB3	2:D:240:ILE:HD12	1.69	0.73
1:C:706:THR:HB	1:C:707:PRO:HD2	1.71	0.71
2:D:468:MET:HE2	2:D:471:ALA:HA	1.70	0.71
2:B:554:VAL:HG12	2:B:558:LYS:HD2	1.72	0.70
3:A:800:B12:H353	3:A:800:B12:H302	1.73	0.70
1:A:706:THR:HB	1:A:707:PRO:HD2	1.73	0.70
1:C:503:ARG:HD2	1:C:508:VAL:HG21	1.74	0.69
1:A:247:GLU:HB3	3:A:800:B12:H532	1.74	0.68
2:B:579:LEU:HG	2:B:583:LYS:HD2	1.74	0.68
3:C:800:B12:H353	3:C:800:B12:H302	1.75	0.67
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.43	0.67
2:D:564:VAL:HG22	2:D:592:ALA:HB3	1.78	0.65
2:B:617:LEU:HD22	2:B:621:MET:HE1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.79	0.64
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.80	0.64
2:D:579:LEU:HG	2:D:583:LYS:HD2	1.80	0.64
2:B:507:VAL:HG21	2:B:636:VAL:HG22	1.81	0.62
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.82	0.61
4:A:801[A]:SCA:NP2	4:A:801[A]:SCA:H92	2.15	0.61
1:C:247:GLU:HB3	3:C:800:B12:H532	1.82	0.61
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.83	0.60
1:C:599:ARG:HG2	1:C:649:VAL:HA	1.83	0.60
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.84	0.60
4:C:801[A]:SCA:NP2	4:C:801[A]:SCA:CP9	2.63	0.60
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.84	0.59
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.84	0.59
2:D:554:VAL:HG12	2:D:558:LYS:HD2	1.84	0.58
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.84	0.57
2:D:532:SER:HB3	2:D:533:PRO:HD3	1.87	0.57
1:A:599:ARG:HG2	1:A:649:VAL:HG12	1.86	0.56
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.88	0.56
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.87	0.56
2:D:197:LEU:HB2	2:D:233:ALA:HA	1.88	0.56
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.87	0.56
3:C:800:B12:H353	3:C:800:B12:C30	2.37	0.55
1:A:359:HIS:CE1	1:A:401:ASP:H	2.24	0.55
1:C:139:ALA:HB1	3:C:800:B12:H362	1.89	0.55
1:C:359:HIS:CE1	1:C:401:ASP:H	2.23	0.55
3:A:800:B12:H351	3:A:800:B12:H372	1.89	0.55
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.87	0.55
1:A:599:ARG:HG2	1:A:649:VAL:HA	1.89	0.54
1:A:120:PRO:HG3	1:A:132:VAL:HB	1.89	0.54
3:A:800:B12:H351	3:A:800:B12:H362	1.89	0.54
3:C:800:B12:H261	6:C:803:5AD:H3'	1.90	0.53
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.73	0.53
2:D:390:VAL:HG12	2:D:392:ILE:HG23	1.90	0.53
1:C:577:THR:HG22	1:C:580:VAL:H	1.74	0.53
1:A:706:THR:HB	1:A:707:PRO:CD	2.37	0.53
2:B:513:VAL:HG13	2:B:564:VAL:HG12	1.90	0.53
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.91	0.52
2:D:272:THR:HB	2:D:275:GLU:H	1.75	0.52
2:D:507:VAL:HG12	2:D:509:GLU:H	1.75	0.52
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.92	0.52
2:D:27:PHE:HB3	2:D:28:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:HB1	3:A:800:B12:H362	1.92	0.52
1:A:89:TYR:CE2	5:A:802[B]:MCA:HS2	2.45	0.51
2:D:180:VAL:HG13	2:D:197:LEU:HD21	1.93	0.51
1:C:444:MET:HE2	1:C:566:ILE:HG22	1.92	0.50
2:B:513:VAL:HG23	2:B:540:ILE:HG21	1.93	0.50
2:D:80:ASP:HB3	2:D:407:SER:HB2	1.92	0.50
2:D:518:LEU:HD22	2:D:581:VAL:HG21	1.93	0.50
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.94	0.50
1:A:512:LEU:HD21	1:A:543:ALA:HB1	1.94	0.49
2:B:613:ILE:HG22	2:B:615:GLY:H	1.77	0.49
1:C:138:MET:SD	1:C:485:ASN:HB2	2.52	0.49
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.95	0.49
1:A:683:THR:HG21	1:A:718:LEU:HD13	1.93	0.49
3:A:800:B12:O7R	3:A:800:B12:H2B	2.13	0.49
1:C:610:HIS:NE2	3:C:800:B12:H202	2.28	0.48
1:A:484:ASP:HB3	1:A:487:THR:HG22	1.96	0.48
2:D:219:ASP:HA	2:D:222:ARG:NH2	2.27	0.48
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.95	0.48
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.78	0.48
2:D:331:LEU:HD13	2:D:365:GLN:HB3	1.95	0.48
1:C:484:ASP:HB3	1:C:487:THR:HG22	1.94	0.48
1:C:79:TYR:HB3	1:C:397:THR:HB	1.95	0.48
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.96	0.47
1:A:444:MET:HE2	1:A:566:ILE:HG22	1.96	0.47
3:A:800:B12:H261	6:A:803:5AD:H3'	1.97	0.47
2:D:617:LEU:HD22	2:D:621:MET:HE1	1.96	0.47
3:A:800:B12:H601	3:A:800:B12:H252	1.97	0.47
4:A:801[A]:SCA:OS1	4:A:801[A]:SCA:CS4	2.60	0.47
1:C:638:GLU:HA	1:C:671:GLU:HG2	1.96	0.47
1:A:374:LEU:HB2	1:A:481:LEU:HD23	1.97	0.47
1:A:599:ARG:HH21	1:A:647:ALA:HB1	1.80	0.47
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.97	0.47
4:C:801[A]:SCA:H92	4:C:801[A]:SCA:HN2	1.77	0.47
1:C:528:ASP:HA	1:C:533:LYS:HE3	1.97	0.46
1:C:706:THR:HB	1:C:707:PRO:CD	2.44	0.46
2:B:538:ALA:HB2	2:B:627:LEU:HD13	1.96	0.46
3:A:800:B12:HM63	3:A:800:B12:HM51	1.78	0.46
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.50	0.46
1:A:372:ILE:HD13	1:A:478:LEU:HD23	1.96	0.46
1:C:252:ALA:O	1:C:256:MET:HG3	2.16	0.46
3:A:800:B12:H2B	3:A:800:B12:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ASN:ND2	2:B:323:ASN:HD21	2.11	0.45
1:C:405:GLY:O	1:C:406:SER:C	2.59	0.45
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.51	0.45
1:A:577:THR:HG22	1:A:580:VAL:H	1.81	0.45
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.98	0.45
2:D:232:ARG:HD2	2:D:321:ARG:HH21	1.81	0.45
3:C:800:B12:HM63	3:C:800:B12:HM51	1.79	0.45
1:C:89:TYR:CE2	5:C:802[B]:MCA:HS2	2.51	0.45
1:A:503:ARG:HD2	1:A:508:VAL:HG21	1.98	0.45
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.47	0.45
2:D:176:ALA:HB1	2:D:197:LEU:HD22	1.98	0.45
8:C:807:HOH:O	2:D:42:VAL:HG21	2.16	0.45
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.48	0.44
2:D:133:VAL:HG23	2:D:380:ARG:HD2	1.99	0.44
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.99	0.44
1:A:138:MET:SD	1:A:485:ASN:HB2	2.58	0.44
2:B:92:PRO:O	2:B:93:PHE:HB2	2.18	0.44
2:D:252:LEU:HD11	2:D:300:LEU:HA	1.99	0.44
2:D:267:VAL:HA	2:D:271:PHE:O	2.18	0.44
1:A:589:GLU:HG3	1:A:723:ARG:NH1	2.33	0.44
2:B:515:LEU:HD12	2:B:528:GLU:HG2	2.00	0.44
2:D:333:ARG:HH21	2:D:498:GLU:HB3	1.82	0.44
1:A:448:GLU:HG2	1:A:569:VAL:HG21	1.99	0.43
1:C:215:GLN:HB3	1:C:216:PRO:CD	2.47	0.43
1:C:441:ILE:HB	1:C:442:PRO:HD3	2.00	0.43
3:C:800:B12:C53	3:C:800:B12:H543	2.47	0.43
3:A:800:B12:H372	3:A:800:B12:C35	2.49	0.43
1:C:250:ALA:HB2	1:C:446:ILE:HG12	2.00	0.43
1:A:589:GLU:HG3	1:A:723:ARG:HH12	1.84	0.43
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.39	0.43
2:D:208:GLN:O	2:D:486:LYS:HB2	2.19	0.43
4:C:801[A]:SCA:OS1	4:C:801[A]:SCA:CS4	2.66	0.43
1:A:577:THR:HA	1:A:578:PRO:HD3	1.90	0.43
1:C:406:SER:HB3	1:C:409:VAL:HB	2.01	0.42
2:D:429:MET:HE3	2:D:433:VAL:HG23	2.01	0.42
1:A:597:ARG:HH11	1:A:597:ARG:HG2	1.84	0.42
1:C:597:ARG:HG2	1:C:597:ARG:HH11	1.84	0.42
1:A:252:ALA:O	1:A:256:MET:HG3	2.20	0.42
1:A:606:GLY:O	1:A:634:PHE:HA	2.19	0.42
2:B:331:LEU:HD13	2:B:365:GLN:HB3	2.02	0.42
1:C:541:ALA:O	1:C:542:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:TYR:O	2:D:171:ASP:HB2	2.20	0.42
3:A:800:B12:H353	3:A:800:B12:C30	2.45	0.42
2:B:272:THR:HB	2:B:275:GLU:H	1.84	0.42
2:B:325:ILE:HD11	2:B:361:LEU:HD21	2.02	0.42
2:B:631:LEU:HD22	2:B:636:VAL:HG11	2.02	0.41
1:C:25:PHE:HB2	2:D:87:TYR:HB3	2.02	0.41
1:C:63:THR:HB	8:C:908:HOH:O	2.19	0.41
1:A:10:VAL:HG11	2:B:310:VAL:HG21	2.03	0.41
1:A:668:LEU:HD13	1:A:682:ILE:HG12	2.02	0.41
2:D:613:ILE:HG22	2:D:615:GLY:H	1.85	0.41
2:B:517:CYS:HA	2:B:568:CYS:O	2.21	0.41
1:A:602:LEU:HD11	1:A:617:ILE:HG22	2.03	0.41
1:C:668:LEU:HD13	1:C:682:ILE:HG12	2.02	0.41
2:D:86:GLY:HA3	8:D:648:HOH:O	2.20	0.41
1:A:213:PRO:HD2	1:A:216:PRO:HG2	2.02	0.41
1:A:215:GLN:HB3	1:A:216:PRO:CD	2.50	0.41
2:B:48:PRO:HG2	2:B:51:LYS:HB2	2.03	0.41
2:B:267:VAL:HA	2:B:271:PHE:O	2.21	0.41
2:B:567:LEU:HD11	2:B:582:ALA:HB2	2.02	0.41
1:C:203:GLU:OE2	1:C:207:ARG:HD3	2.21	0.41
1:C:683:THR:HG22	1:C:703:GLU:HB2	2.03	0.41
1:C:710:VAL:HB	1:C:713:GLU:HB2	2.03	0.41
1:A:24:ARG:HG2	1:A:24:ARG:HH11	1.86	0.40
1:A:216:PRO:HB3	1:A:556:PHE:CD1	2.55	0.40
1:C:8:ASP:HA	2:D:421:GLN:HG2	2.03	0.40
1:A:617:ILE:HG21	3:A:800:B12:HM52	2.03	0.40
1:A:638:GLU:HG3	1:A:671:GLU:OE2	2.20	0.40
3:A:800:B12:C42	3:A:800:B12:H363	2.52	0.40
1:C:243:TYR:CE2	1:C:247:GLU:HG3	2.56	0.40
1:C:328:HIS:HB2	4:C:801[A]:SCA:H52	2.04	0.40
2:D:592:ALA:HB2	2:D:633:ILE:HG21	2.03	0.40
2:B:129:LEU:HD21	2:B:136:LEU:HD21	2.04	0.40
2:B:272:THR:HG22	8:B:863:HOH:O	2.20	0.40
2:B:284:VAL:HG21	2:B:297:LEU:HD22	2.02	0.40
3:A:800:B12:H362	3:A:800:B12:C35	2.52	0.40
2:B:554:VAL:HG21	2:B:584:ALA:HB1	2.03	0.40
3:C:800:B12:H351	3:C:800:B12:H372	2.03	0.40
2:B:431:LYS:HD2	2:B:431:LYS:HA	1.98	0.40
2:D:517:CYS:HB2	2:D:545:VAL:O	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	724/727 (100%)	697 (96%)	27 (4%)	0	100	100
1	C	724/727 (100%)	687 (95%)	37 (5%)	0	100	100
2	B	617/637 (97%)	591 (96%)	24 (4%)	2 (0%)	36	42
2	D	617/637 (97%)	584 (95%)	31 (5%)	2 (0%)	36	42
All	All	2682/2728 (98%)	2559 (95%)	119 (4%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	171	ASP
2	D	269	GLN
2	B	269	GLN
2	B	171	ASP

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	572/590 (97%)	554 (97%)	18 (3%)	35	48
1	C	572/590 (97%)	557 (97%)	15 (3%)	40	55
2	B	481/509 (94%)	463 (96%)	18 (4%)	30	41
2	D	481/509 (94%)	460 (96%)	21 (4%)	25	34
All	All	2106/2198 (96%)	2034 (97%)	72 (3%)	32	44

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	14	ASN
1	A	24	ARG
1	A	93	SER
1	A	96	LYS
1	A	127	SER
1	A	131	ARG
1	A	202	LYS
1	A	365	THR
1	A	414	TRP
1	A	430	VAL
1	A	533	LYS
1	A	577	THR
1	A	588	GLU
1	A	597	ARG
1	A	619	THR
1	A	668	LEU
1	A	723	ARG
2	B	83	LYS
2	B	119	LYS
2	B	155	SER
2	B	186	SER
2	B	191	LYS
2	B	199	LEU
2	B	216	VAL
2	B	228	SER
2	B	272	THR
2	B	334	GLU
2	B	410	ARG
2	B	418	LYS
2	B	436	GLU
2	B	451	LYS
2	B	515	LEU
2	B	577	GLN
2	B	586	LYS
2	B	638	LYS
1	C	3	THR
1	C	4	LEU
1	C	24	ARG
1	C	96	LYS
1	C	202	LYS
1	C	265	ASP

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Mol	Chain	Res	Type
1	C	318	LYS
1	C	369	ASP
1	C	430	VAL
1	C	482	LYS
1	C	567	SER
1	C	577	THR
1	C	588	GLU
1	C	597	ARG
1	C	668	LEU
2	D	20	THR
2	D	72	ILE
2	D	83	LYS
2	D	119	LYS
2	D	141	ASP
2	D	155	SER
2	D	186	SER
2	D	191	LYS
2	D	216	VAL
2	D	228	SER
2	D	240	ILE
2	D	272	THR
2	D	334	GLU
2	D	410	ARG
2	D	418	LYS
2	D	451	LYS
2	D	577	GLN
2	D	586	LYS
2	D	608	GLU
2	D	617	LEU
2	D	638	LYS

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

Mol	Chain	Res	Type
1	A	14	ASN
1	A	51	ASN
1	A	99	ASN
1	A	313	HIS
1	A	359	HIS
1	A	385	ASN
1	A	462	GLN
1	A	492	GLN

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Mol	Chain	Res	Type
1	A	643	GLN
2	B	323	ASN
2	B	365	GLN
2	B	458	GLN
1	C	14	ASN
1	C	313	HIS
1	C	359	HIS
1	C	385	ASN
1	C	492	GLN
1	C	592	GLN
1	C	635	GLN
1	C	643	GLN
2	D	322	GLN
2	D	323	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](#)

12 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
6	5AD	A	803	-	20,20,20	0.49	0	28,30,30	1.67	5 (17%)
7	GOL	B	639	-	5,5,5	0.34	0	5,5,5	0.68	0
4	SCA	A	801[A]	-	55,57,57	0.91	3 (5%)	78,84,84	1.33	8 (10%)
5	MCA	C	802[B]	-	54,57,57	0.86	1 (1%)	77,85,85	1.11	5 (6%)
7	GOL	D	639	-	5,5,5	0.51	0	5,5,5	0.69	0
3	B12	C	800	1	94,101,101	1.10	9 (9%)	149,166,166	1.75	37 (24%)
6	5AD	C	803	-	20,20,20	0.62	0	28,30,30	1.92	5 (17%)
3	B12	A	800	1	94,101,101	1.19	8 (8%)	149,166,166	1.76	36 (24%)
7	GOL	A	1	-	5,5,5	0.70	0	5,5,5	1.25	1 (20%)
5	MCA	A	802[B]	-	54,57,57	0.95	3 (5%)	77,85,85	1.19	6 (7%)
4	SCA	C	801[A]	-	55,57,57	0.84	2 (3%)	78,84,84	1.38	13 (16%)
7	GOL	C	1	-	5,5,5	0.73	0	5,5,5	1.09	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5AD	A	803	-	-	0/4/20/20	0/3/3/3
7	GOL	B	639	-	-	2/4/4/4	-
4	SCA	A	801[A]	-	-	5/56/72/72	0/3/3/3
5	MCA	C	802[B]	-	-	8/59/75/75	0/3/3/3
7	GOL	D	639	-	-	2/4/4/4	-
3	B12	C	800	1	-	9/56/223/223	0/3/11/11
6	5AD	C	803	-	-	0/4/20/20	0/3/3/3
3	B12	A	800	1	-	11/56/223/223	0/3/11/11
7	GOL	A	1	-	-	0/4/4/4	-
5	MCA	A	802[B]	-	-	7/59/75/75	0/3/3/3
4	SCA	C	801[A]	-	-	8/56/72/72	0/3/3/3
7	GOL	C	1	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C14-N23	4.40	1.41	1.35
3	A	800	B12	C2B-N1B	-3.66	1.31	1.37
5	A	802[B]	MCA	P2-O6	3.32	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C48-C13	3.01	1.61	1.54
5	C	802[B]	MCA	OS4-CS4	-2.84	1.21	1.30
3	C	800	B12	C19-N24	-2.79	1.45	1.49
3	C	800	B12	C54-C17	2.78	1.59	1.54
4	A	801[A]	SCA	P2-O6	2.78	1.62	1.59
3	C	800	B12	C14-N23	2.71	1.38	1.35
3	A	800	B12	C54-C17	2.56	1.58	1.54
3	A	800	B12	C19-N24	-2.49	1.46	1.49
5	A	802[B]	MCA	OS4-CS4	-2.39	1.23	1.30
3	C	800	B12	C2B-N1B	-2.26	1.33	1.37
3	C	800	B12	C55-C17	-2.26	1.49	1.54
3	A	800	B12	C55-C56	2.25	1.58	1.53
3	A	800	B12	P-O2	2.24	1.66	1.59
4	C	801[A]	SCA	OS4-CS4	-2.23	1.23	1.30
3	C	800	B12	C48-C13	2.19	1.59	1.54
4	A	801[A]	SCA	P3-O3'	2.17	1.63	1.59
3	C	800	B12	C46-C12	2.08	1.58	1.54
3	C	800	B12	C55-C56	2.07	1.57	1.53
3	A	800	B12	C7B-C6B	2.06	1.42	1.39
5	A	802[B]	MCA	P3-O3'	2.05	1.63	1.59
4	A	801[A]	SCA	OS4-CS4	-2.05	1.24	1.30
4	C	801[A]	SCA	P1-O11	-2.05	1.45	1.55
3	C	800	B12	C7B-C6B	2.05	1.42	1.39

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C9B-C8B-N1B	5.98	107.95	105.30
6	C	803	5AD	C5'-C4'-C3'	-5.91	109.49	115.70
4	A	801[A]	SCA	OS1-CS1-S	5.14	129.22	122.68
3	A	800	B12	C16-C15-C14	-5.14	113.42	121.26
4	C	801[A]	SCA	CP9-CPA-CP7	-4.84	100.53	108.77
6	A	803	5AD	C5'-C4'-C3'	-4.83	110.62	115.70
3	C	800	B12	C54-C17-C16	-4.82	87.42	112.41
6	C	803	5AD	N3-C2-N1	4.70	135.70	128.58
5	A	802[B]	MCA	CP1-CP2-NP1	-4.58	102.85	112.41
5	A	802[B]	MCA	CP2-NP1-CP3	-4.46	114.53	122.82
3	A	800	B12	C54-C17-C16	-4.44	89.42	112.41
3	C	800	B12	C35-C5-C6	4.29	129.32	122.41
3	C	800	B12	C55-C17-C16	4.28	124.96	116.59
4	C	801[A]	SCA	OS4-CS4-CS3	4.17	127.18	114.00
3	C	800	B12	C16-C15-C14	-4.17	114.90	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C18-C19-N24	4.13	108.54	102.33
4	C	801[A]	SCA	CP1-CP2-NP1	-4.11	103.84	112.41
5	C	802[B]	MCA	CP2-NP1-CP3	-4.08	115.23	122.82
3	A	800	B12	C55-C56-C57	-3.94	102.46	111.25
3	C	800	B12	C55-C17-C18	3.91	118.59	111.12
3	A	800	B12	C53-C15-C14	3.90	126.15	118.42
4	A	801[A]	SCA	CP8-CPA-CPB	3.90	114.66	108.22
3	C	800	B12	C9B-C8B-N1B	3.89	107.03	105.30
3	A	800	B12	C55-C17-C16	3.77	123.96	116.59
3	C	800	B12	C19-N24-C16	3.70	111.33	107.29
3	A	800	B12	C55-C17-C18	3.67	118.12	111.12
3	C	800	B12	C53-C15-C14	3.62	125.58	118.42
3	C	800	B12	O58-C57-N59	3.47	129.84	123.03
4	A	801[A]	SCA	CP1-CP2-NP1	-3.43	105.25	112.41
5	C	802[B]	MCA	CP1-CP2-NP1	-3.42	105.27	112.41
6	A	803	5AD	N3-C2-N1	3.41	133.75	128.58
3	C	800	B12	C18-C19-N24	3.38	107.42	102.33
3	C	800	B12	C7B-C8B-C9B	3.31	126.44	122.47
3	A	800	B12	C13-C14-C15	-3.23	119.41	124.32
4	A	801[A]	SCA	OS1-CS1-CS2	-3.23	120.25	123.98
4	C	801[A]	SCA	OS1-CS1-S	3.22	126.78	122.68
3	C	800	B12	C3-C4-N21	3.21	115.97	111.98
3	C	800	B12	C9-N22-C6	3.18	109.11	105.28
6	C	803	5AD	C2-N3-C4	-3.15	104.13	111.83
3	C	800	B12	C15-C16-N24	3.11	126.85	122.42
4	C	801[A]	SCA	CP9-CPA-CPB	3.06	113.27	108.22
3	C	800	B12	C20-C1-C19	3.05	112.28	109.35
3	A	800	B12	C2-C1-C19	-3.03	113.91	118.61
3	C	800	B12	C2-C1-C19	-3.03	113.91	118.61
3	A	800	B12	C15-C16-N24	3.02	126.72	122.42
5	C	802[B]	MCA	OS1-CS1-S	2.95	127.77	123.80
4	A	801[A]	SCA	CP9-CPA-CP7	-2.93	103.77	108.77
6	A	803	5AD	C5-C4-N3	2.91	130.73	126.72
3	A	800	B12	C13-C14-N23	2.85	112.95	109.09
3	A	800	B12	C1P-N59-C57	-2.84	116.59	122.69
3	C	800	B12	C2P-C1P-N59	-2.82	108.77	112.92
3	A	800	B12	C7-C6-C5	-2.80	123.70	128.07
6	C	803	5AD	C5-C4-N3	2.74	130.49	126.72
3	A	800	B12	C17-C16-C15	-2.73	121.95	126.26
6	A	803	5AD	C2-N3-C4	-2.68	105.29	111.83
5	C	802[B]	MCA	O22-P2-O21	2.64	124.71	112.44
4	C	801[A]	SCA	OS5-CS4-CS3	-2.63	114.74	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C56-C55-C17	-2.62	110.53	115.58
3	C	800	B12	C4B-C5B-C6B	2.62	123.53	119.69
3	C	800	B12	C5M-C5B-C6B	-2.62	115.41	120.76
5	A	802[B]	MCA	OP1-CP3-NP1	-2.57	117.98	123.03
4	A	801[A]	SCA	OS4-CS4-CS3	2.57	122.11	114.00
7	A	1	GOL	C3-C2-C1	-2.56	102.40	111.80
3	A	800	B12	C5M-C5B-C6B	-2.55	115.56	120.76
3	C	800	B12	C25-C2-C1	2.54	117.56	113.75
3	A	800	B12	C20-C1-C19	2.54	111.79	109.35
3	A	800	B12	C18-C17-C16	2.49	103.69	100.69
3	C	800	B12	C56-C55-C17	-2.49	110.79	115.58
3	A	800	B12	C4R-O6R-C1R	-2.48	104.00	109.47
3	C	800	B12	C35-C5-C4	-2.47	111.79	116.79
3	C	800	B12	C7B-C8B-N1B	-2.46	126.53	131.39
4	C	801[A]	SCA	CP5-NP2-CP6	-2.45	118.14	122.55
3	A	800	B12	C19-N24-C16	2.44	109.96	107.29
3	C	800	B12	O51-C50-C49	-2.44	113.68	121.04
5	A	802[B]	MCA	CP9-CPA-CP7	2.43	112.91	108.77
3	C	800	B12	C55-C56-C57	-2.42	105.85	111.25
4	A	801[A]	SCA	CS2-CS1-S	-2.42	110.52	113.40
3	A	800	B12	C7-C6-N22	2.40	112.31	107.94
5	C	802[B]	MCA	OS5-CS4-CS2	-2.39	112.57	122.72
3	A	800	B12	C8B-C9B-N3B	-2.38	107.43	110.00
3	A	800	B12	C41-C8-C9	-2.37	107.04	111.19
4	C	801[A]	SCA	CP8-CPA-CP9	2.37	113.92	109.20
3	C	800	B12	C54-C17-C55	-2.35	105.35	109.27
3	C	800	B12	C17-C16-C15	-2.32	122.59	126.26
3	A	800	B12	C25-C2-C3	2.31	118.79	112.91
3	A	800	B12	C31-C30-C3	-2.31	108.10	114.65
3	A	800	B12	C48-C13-C12	-2.31	109.92	116.52
3	A	800	B12	C9-C10-C11	-2.30	122.68	125.97
3	C	800	B12	C41-C8-C9	-2.30	107.18	111.19
3	A	800	B12	C31-C32-N33	2.29	123.82	116.49
5	A	802[B]	MCA	CP8-CPA-CPB	2.29	112.00	108.22
3	A	800	B12	C7B-C8B-N1B	-2.28	126.88	131.39
3	C	800	B12	O58-C57-C56	-2.28	117.89	122.02
5	A	802[B]	MCA	O22-P2-O21	2.28	123.05	112.44
4	C	801[A]	SCA	CP8-CPA-CPB	2.27	111.98	108.22
3	C	800	B12	O44-C43-N45	-2.27	116.48	122.53
3	A	800	B12	C7B-C8B-C9B	2.24	125.17	122.47
6	A	803	5AD	O4'-C1'-N9	-2.24	103.79	108.09
3	C	800	B12	C56-C57-N59	-2.23	112.27	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801[A]	SCA	OS5-CS4-CS3	-2.22	116.06	123.09
3	A	800	B12	C9-N22-C6	2.20	107.92	105.28
4	C	801[A]	SCA	O22-P2-O21	2.19	122.61	112.44
3	C	800	B12	C18-C17-C16	2.17	103.30	100.69
4	C	801[A]	SCA	CP2-NP1-CP3	-2.16	118.81	122.82
3	C	800	B12	C9B-C4B-C5B	-2.13	116.87	120.83
3	C	800	B12	O5-P-O4	2.13	122.37	112.44
7	C	1	GOL	C3-C2-C1	-2.13	103.99	111.80
3	A	800	B12	C3-C4-N21	2.08	114.56	111.98
3	A	800	B12	O6R-C1R-C2R	-2.07	102.18	106.62
3	A	800	B12	O5-P-O4	2.07	122.06	112.44
3	C	800	B12	C7-C6-C5	-2.07	124.84	128.07
4	C	801[A]	SCA	CP4-CP5-NP2	2.06	116.39	112.00
3	C	800	B12	C8-C9-C10	-2.06	118.94	123.33
3	A	800	B12	C3-C4-C5	-2.06	120.38	123.82
6	C	803	5AD	C4-N9-C8	2.05	107.89	105.74
4	C	801[A]	SCA	OS4-CS4-OS5	-2.05	118.07	123.33
3	C	800	B12	C2-C26-C27	-2.00	109.62	115.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C42-C41-C8-C9
3	C	800	B12	C2R-C1R-N1B-C2B
4	A	801[A]	SCA	OS1-CS1-S-CP1
4	A	801[A]	SCA	CS2-CS1-S-CP1
4	C	801[A]	SCA	OS1-CS1-S-CP1
4	C	801[A]	SCA	CS2-CS1-S-CP1
4	C	801[A]	SCA	CS1-CS2-CS3-CS4
5	A	802[B]	MCA	CP9-CPA-CPB-O7
5	A	802[B]	MCA	CP8-CPA-CPB-O7
3	A	800	B12	C42-C41-C8-C9
3	A	800	B12	C16-C17-C55-C56
3	C	800	B12	C16-C17-C55-C56
7	B	639	GOL	C1-C2-C3-O3
7	C	1	GOL	O1-C1-C2-C3
7	D	639	GOL	C1-C2-C3-O3
3	A	800	B12	C2R-C1R-N1B-C8B
3	C	800	B12	C2R-C1R-N1B-C8B
7	B	639	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	D	639	GOL	O2-C2-C3-O3
7	C	1	GOL	O1-C1-C2-O2
3	A	800	B12	O6R-C1R-N1B-C8B
3	C	800	B12	O6R-C1R-N1B-C8B
5	A	802[B]	MCA	P2-O6-P1-O12
5	C	802[B]	MCA	CP8-CPA-CPB-O7
3	A	800	B12	C30-C31-C32-N33
5	A	802[B]	MCA	CP7-CPA-CPB-O7
3	A	800	B12	C30-C31-C32-O34
5	C	802[B]	MCA	P2-O6-P1-O12
4	A	801[A]	SCA	CS1-CS2-CS3-CS4
3	C	800	B12	C30-C31-C32-N33
5	A	802[B]	MCA	OS1-CS1-CS2-CS3
4	C	801[A]	SCA	CS2-CS3-CS4-OS5
5	A	802[B]	MCA	S-CS1-CS2-CS4
5	C	802[B]	MCA	S-CS1-CS2-CS4
3	A	800	B12	C2P-O3-P-O4
3	A	800	B12	C2P-O3-P-O5
3	C	800	B12	C2P-O3-P-O4
3	C	800	B12	C2P-O3-P-O5
4	A	801[A]	SCA	P2-O6-P1-O11
5	A	802[B]	MCA	P2-O6-P1-O11
5	C	802[B]	MCA	P2-O6-P1-O11
5	C	802[B]	MCA	OS1-CS1-CS2-CS3
3	A	800	B12	C3-C30-C31-C32
4	A	801[A]	SCA	CP9-CPA-CPB-O7
4	C	801[A]	SCA	CP9-CPA-CPB-O7
5	C	802[B]	MCA	CP9-CPA-CPB-O7
5	C	802[B]	MCA	CP6-CP7-CPA-CPB
3	C	800	B12	C30-C31-C32-O34
4	C	801[A]	SCA	CS2-CS3-CS4-OS4
5	C	802[B]	MCA	C4'-C5'-O5'-P1
3	A	800	B12	C55-C56-C57-O58
4	C	801[A]	SCA	NP2-CP6-CP7-OP3
4	C	801[A]	SCA	P2-O6-P1-O11

There are no ring outliers.

8 monomers are involved in 37 short contacts:

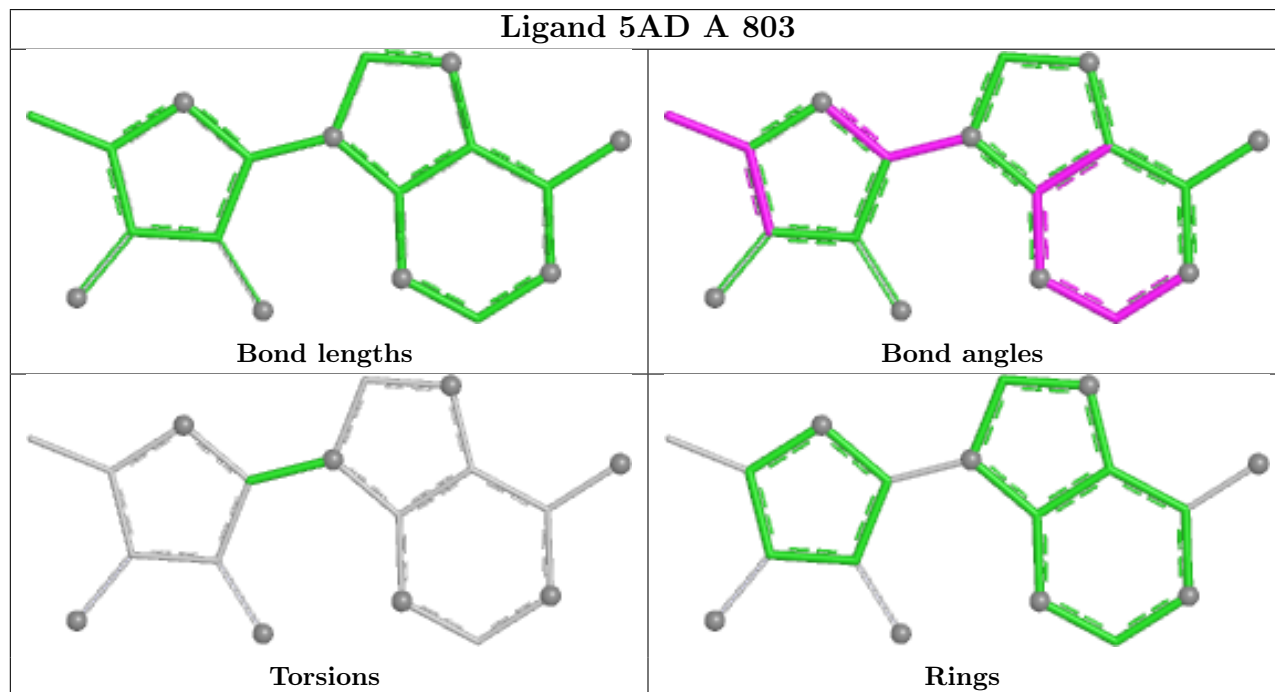
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	803	5AD	1	0
4	A	801[A]	SCA	2	0

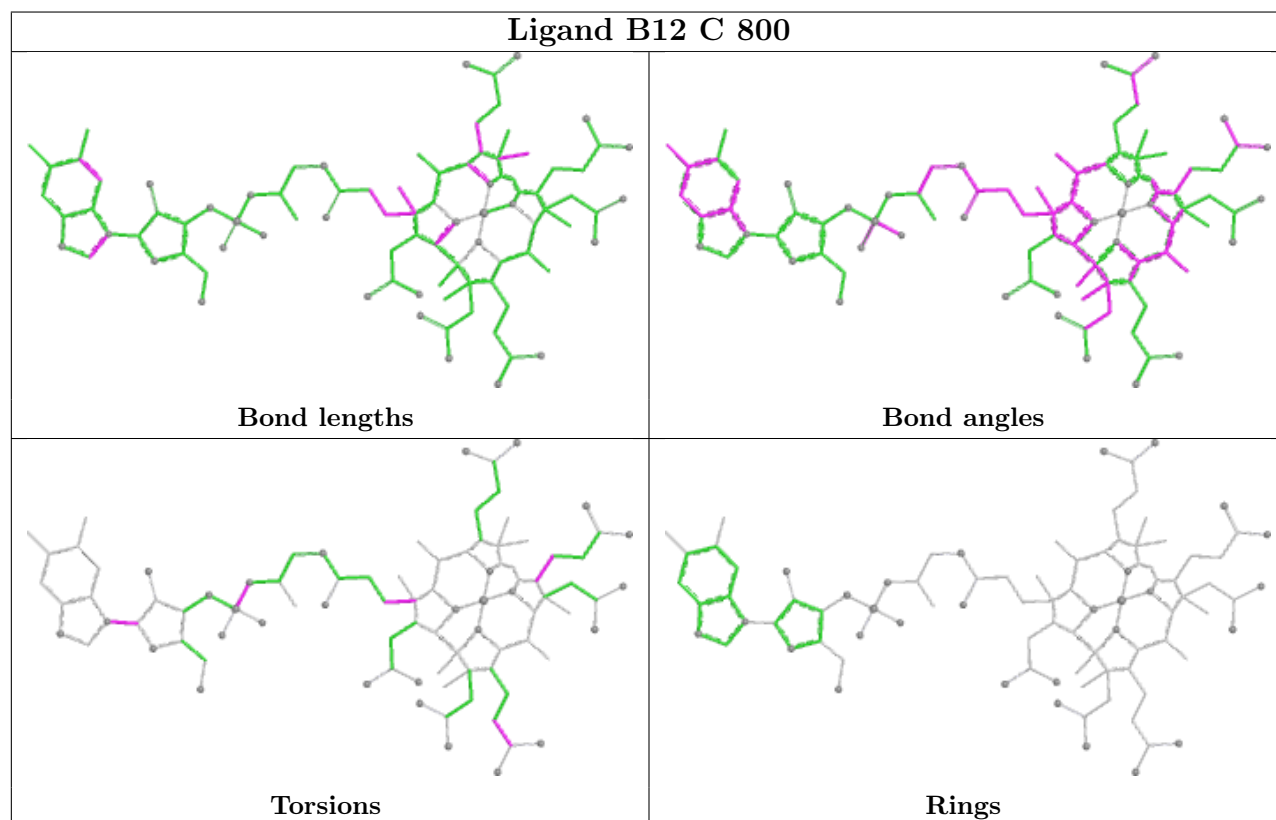
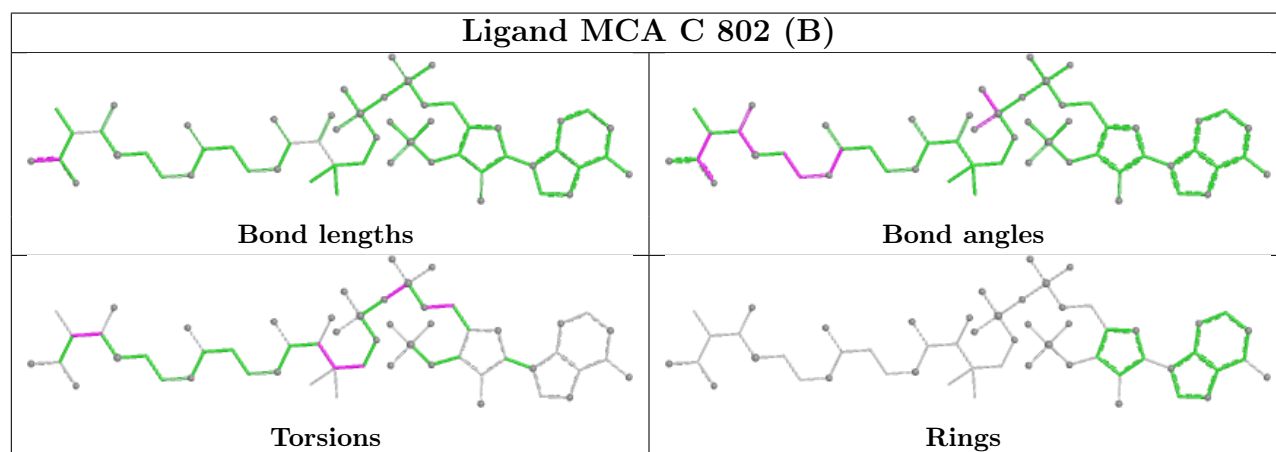
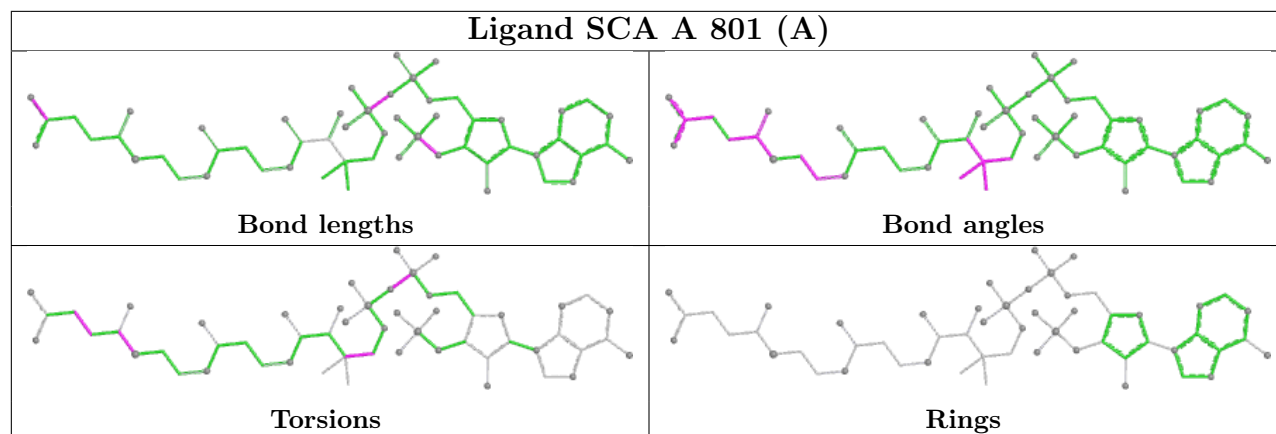
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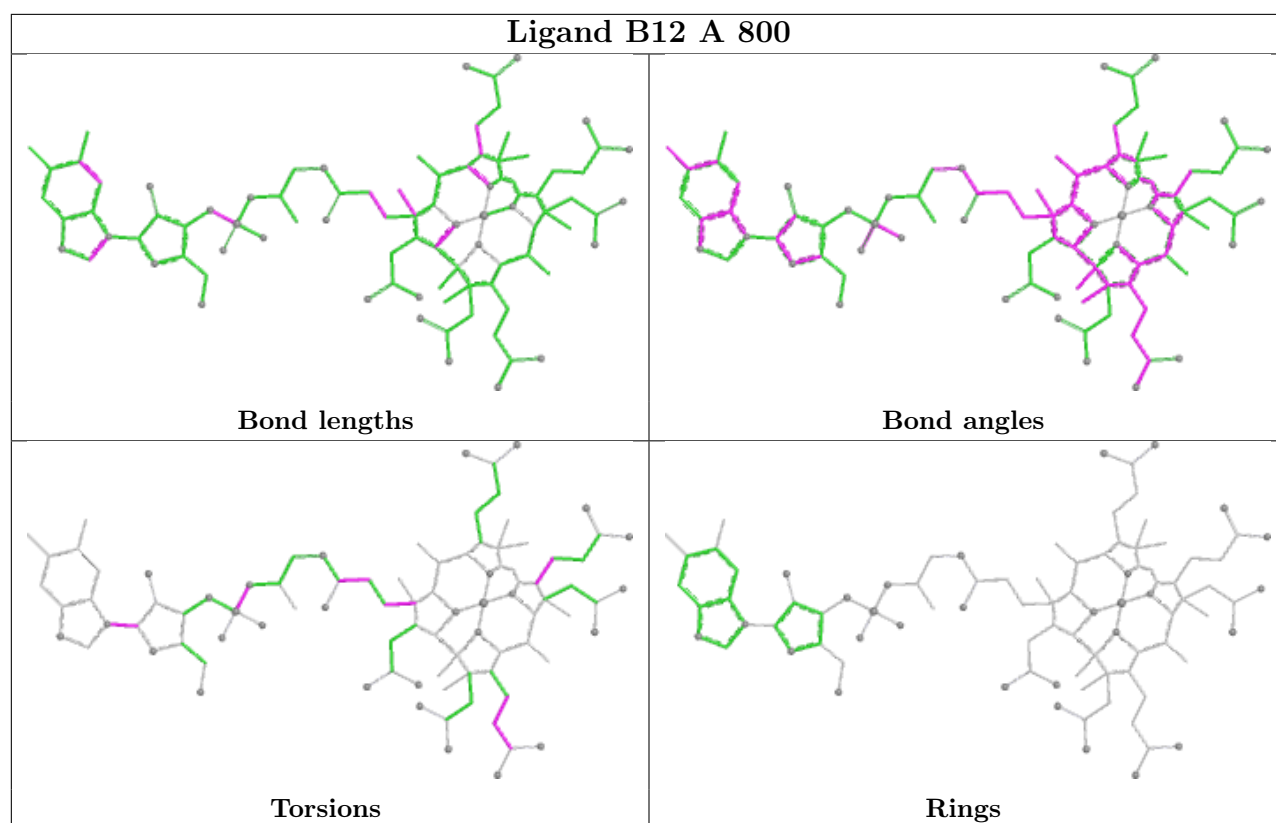
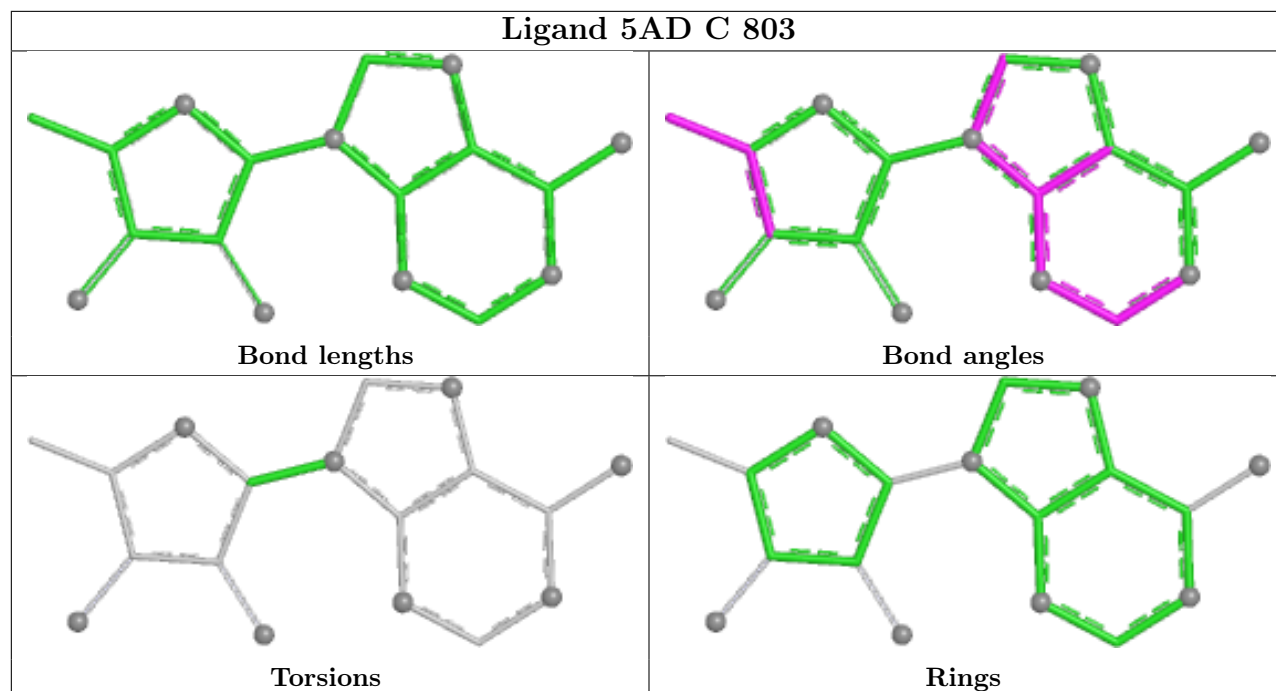
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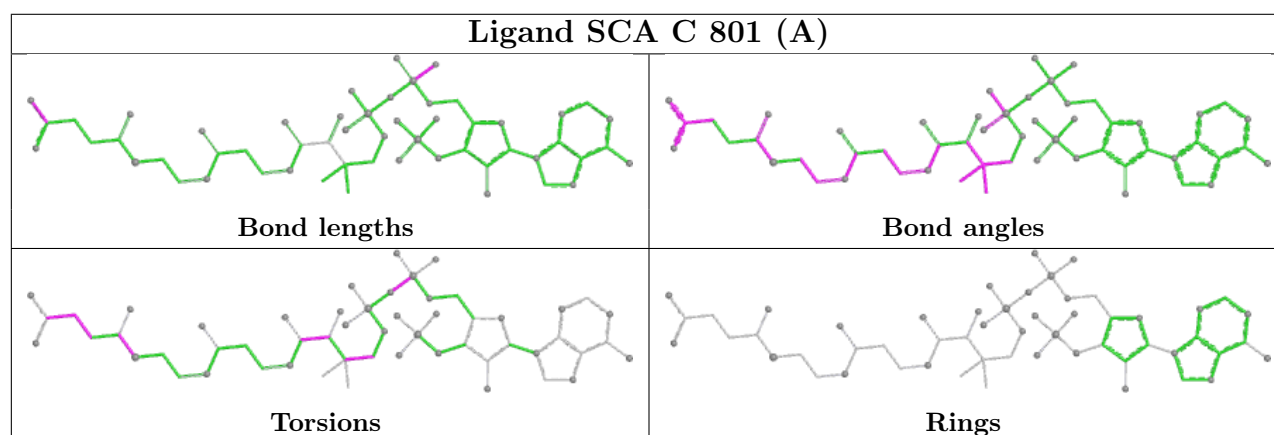
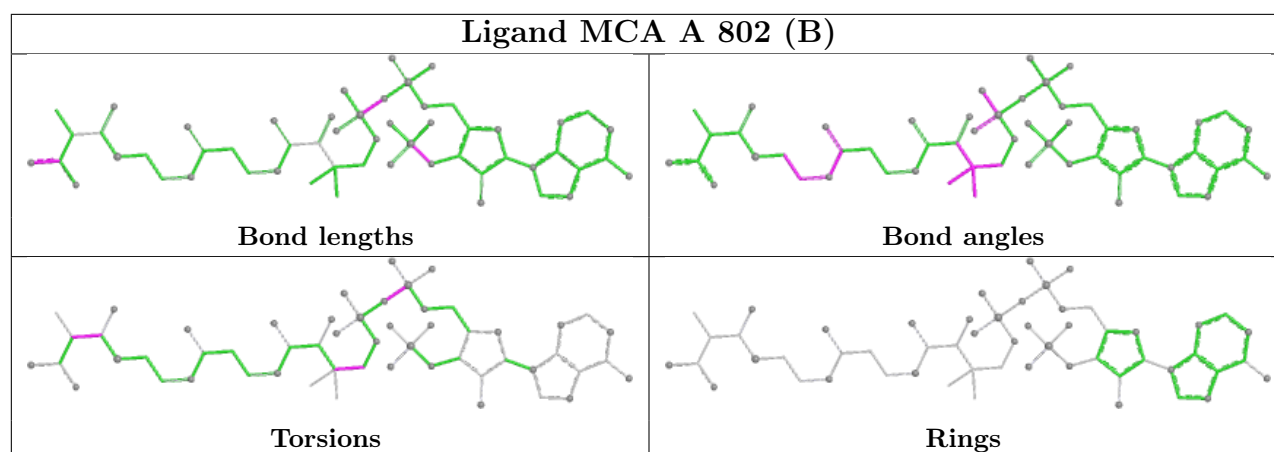
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	802[B]	MCA	1	0
3	C	800	B12	11	0
6	C	803	5AD	1	0
3	A	800	B12	17	0
5	A	802[B]	MCA	1	0
4	C	801[A]	SCA	5	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/727 (99%)	-0.04	8 (1%) 78 76	12, 30, 54, 90	0
1	C	726/727 (99%)	0.03	15 (2%) 63 60	11, 30, 54, 90	0
2	B	619/637 (97%)	0.48	30 (4%) 35 32	16, 42, 71, 103	0
2	D	619/637 (97%)	0.70	55 (8%) 15 13	18, 43, 71, 103	0
All	All	2690/2728 (98%)	0.27	108 (4%) 42 39	11, 35, 66, 103	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	107	TRP	5.4
2	B	107	TRP	4.6
1	C	728	ALA	4.6
1	C	23	ARG	4.5
2	B	106	ALA	4.1
1	A	574	VAL	3.9
2	B	638	LYS	3.9
2	D	106	ALA	3.7
1	C	574	VAL	3.7
2	D	267	VAL	3.7
2	B	185	ARG	3.7
2	D	185	ARG	3.6
2	D	638	LYS	3.4
1	A	3	THR	3.4
2	D	305	ALA	3.4
1	A	728	ALA	3.3
2	D	637	ALA	3.2
2	D	272	THR	3.2
2	D	146	ALA	3.1
1	C	576	ASN	3.0
2	B	150	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	183	TYR	2.9
2	D	178	ALA	2.9
1	C	573	GLU	2.9
2	B	230	ASP	2.9
2	B	637	ALA	2.9
2	D	188	LYS	2.8
1	C	3	THR	2.8
2	B	105	ASP	2.8
2	D	20	THR	2.8
2	D	25	GLY	2.7
2	B	635	GLY	2.7
2	D	173	GLY	2.7
1	A	573	GLU	2.7
2	D	150	LEU	2.7
1	A	576	ASN	2.7
1	C	4	LEU	2.7
2	D	105	ASP	2.6
2	B	636	VAL	2.6
2	B	487	GLY	2.6
2	D	182	VAL	2.6
2	D	633	ILE	2.6
2	B	20	THR	2.6
2	D	227	PHE	2.6
2	D	573	VAL	2.6
2	B	183	TYR	2.5
2	D	217	LEU	2.5
2	B	190	ALA	2.5
2	D	189	PRO	2.5
2	B	188	LYS	2.4
2	D	274	THR	2.4
2	D	158	LEU	2.4
2	D	266	LEU	2.4
2	D	184	GLU	2.4
2	B	272	THR	2.4
2	D	263	VAL	2.4
2	D	507	VAL	2.3
2	D	159	LEU	2.3
1	C	25	PHE	2.3
1	A	4	LEU	2.3
1	C	575	LYS	2.3
2	D	229	PRO	2.3
2	D	635	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	501	ALA	2.2
2	B	140	VAL	2.2
2	B	619	MET	2.2
1	C	510	ALA	2.2
2	B	225	ALA	2.2
2	D	190	ALA	2.2
2	D	202	ILE	2.2
2	D	216	VAL	2.2
2	D	636	VAL	2.2
2	D	311	PHE	2.2
1	C	16	PRO	2.2
2	B	587	ALA	2.2
2	D	91	ALA	2.2
2	D	151	ASP	2.2
2	D	221	VAL	2.2
2	D	487	GLY	2.2
1	C	407	ALA	2.2
1	C	577	THR	2.2
2	B	588	ALA	2.2
2	D	426	LEU	2.1
2	B	501	MET	2.1
2	B	575	ALA	2.1
2	D	587	ALA	2.1
1	A	575	LYS	2.1
2	B	171	ASP	2.1
2	B	373	ASP	2.1
2	D	192	ASP	2.1
2	D	133	VAL	2.1
2	B	207	LEU	2.1
1	A	5	PRO	2.1
2	D	153	VAL	2.1
2	D	234	VAL	2.1
2	B	176	ALA	2.1
2	D	176	ALA	2.1
2	D	607	ALA	2.1
2	B	170	TYR	2.1
2	B	179	LEU	2.0
2	D	193	LEU	2.0
2	D	318	ARG	2.0
2	D	155	SER	2.0
2	D	210	THR	2.0
1	C	511	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	144	ALA	2.0
2	D	276	ALA	2.0
2	B	224	LEU	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](#)

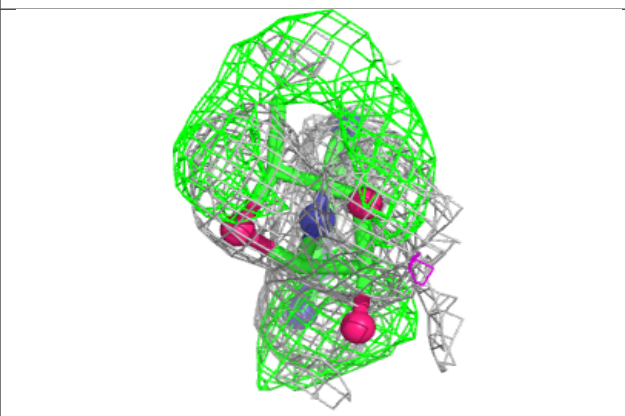
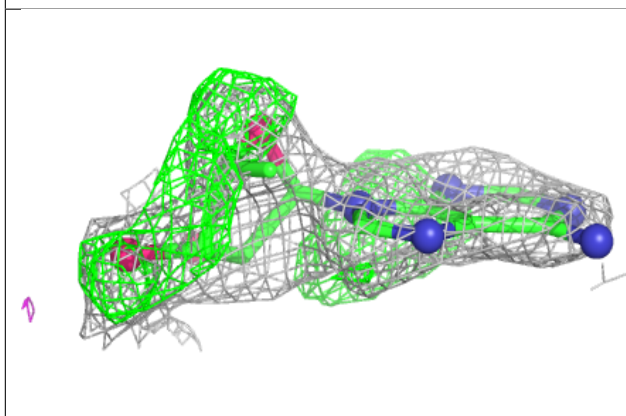
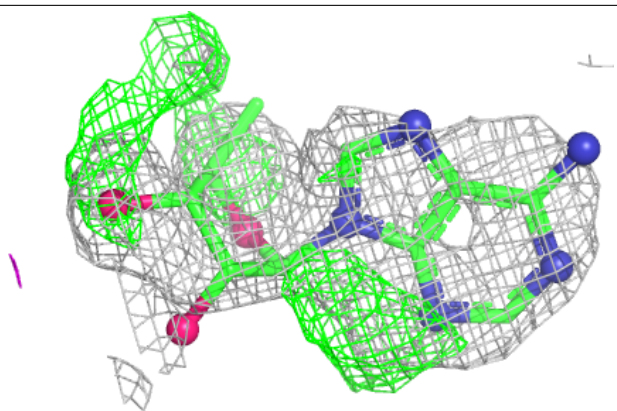
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	5AD	A	803	18/18	0.76	0.28	27,32,35,38	18
6	5AD	C	803	18/18	0.77	0.26	17,30,37,37	18
7	GOL	B	639	6/6	0.79	0.16	37,47,49,49	0
7	GOL	C	1	6/6	0.80	0.13	30,36,38,41	0
7	GOL	D	639	6/6	0.81	0.16	50,53,56,58	0
7	GOL	A	1	6/6	0.83	0.14	28,35,38,42	0
5	MCA	C	802[B]	55/55	0.96	0.07	12,21,25,26	55
5	MCA	A	802[B]	55/55	0.97	0.06	10,20,25,25	55
3	B12	A	800	91/91	0.97	0.06	11,20,28,29	0
4	SCA	A	801[A]	55/55	0.97	0.06	6,20,27,30	55
4	SCA	C	801[A]	55/55	0.97	0.06	7,19,24,26	55
3	B12	C	800	91/91	0.98	0.05	10,18,26,30	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.

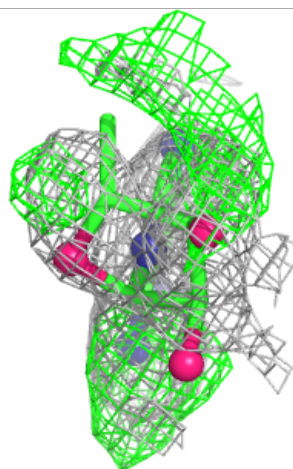
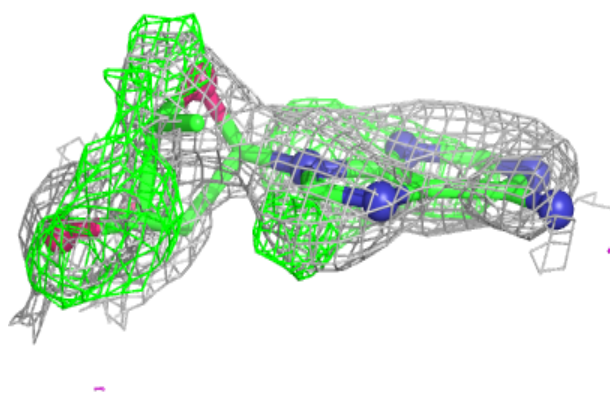
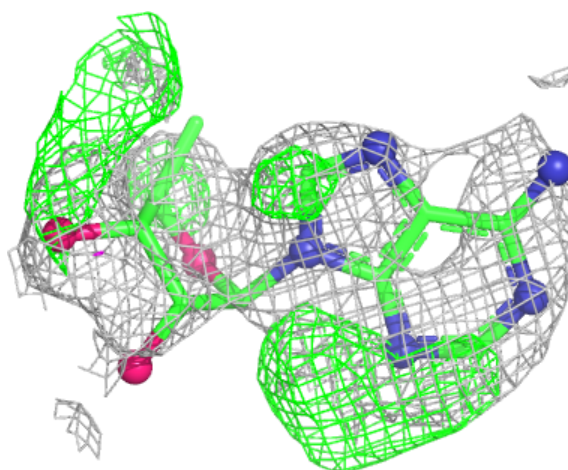
Electron density around 5AD A 803:

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



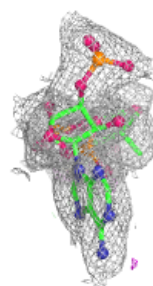
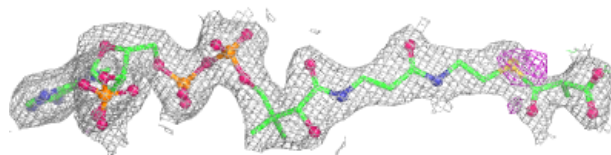
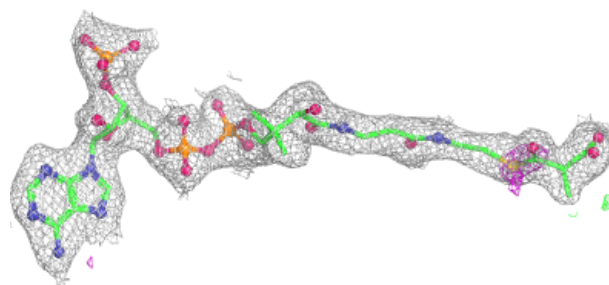
Electron density around 5AD C 803:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

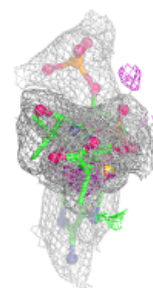
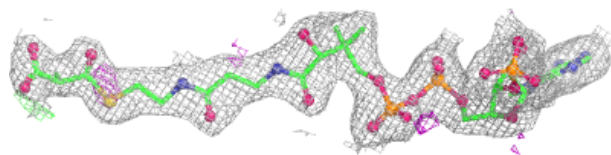
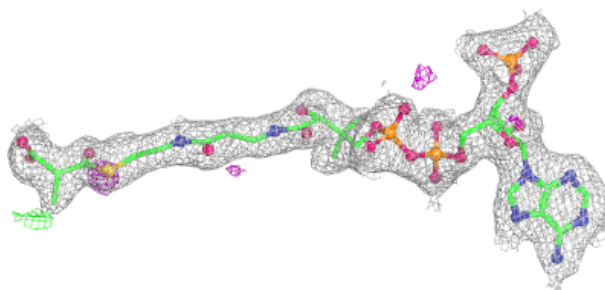


Electron density around MCA C 802 (B):

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and green (positive)

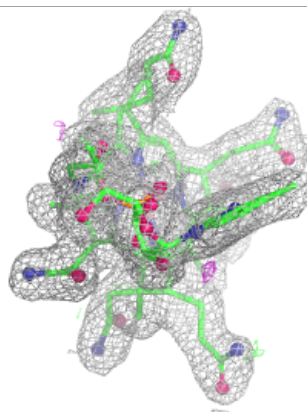
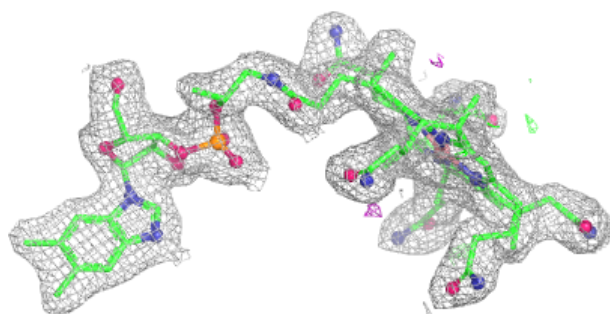
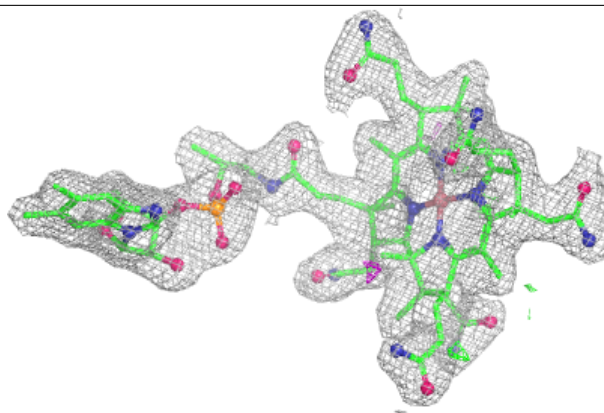
**Electron density around MCA A 802 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

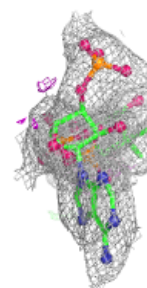
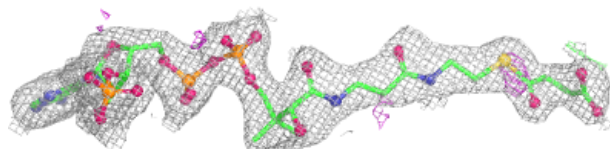
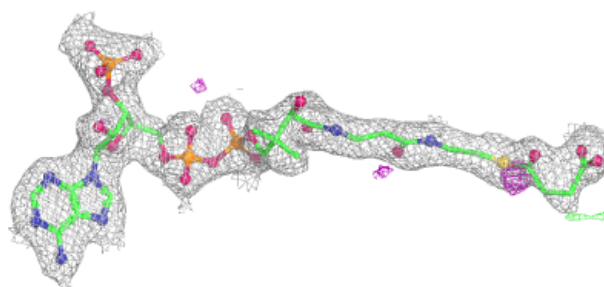


Electron density around B12 A 800:

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

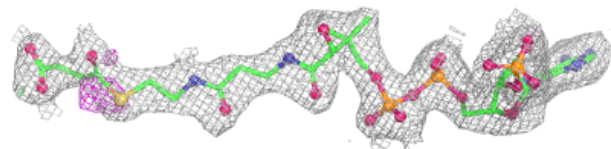
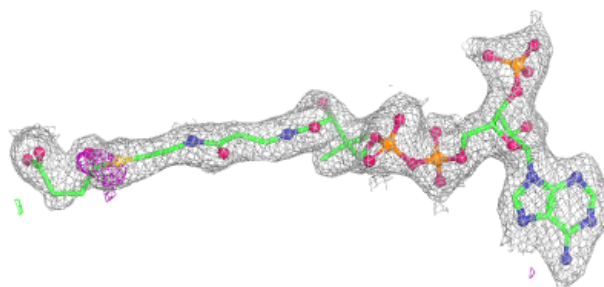
**Electron density around SCA A 801 (A):**

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

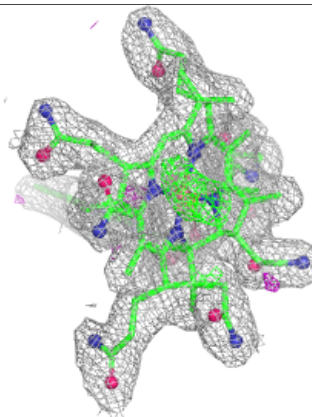
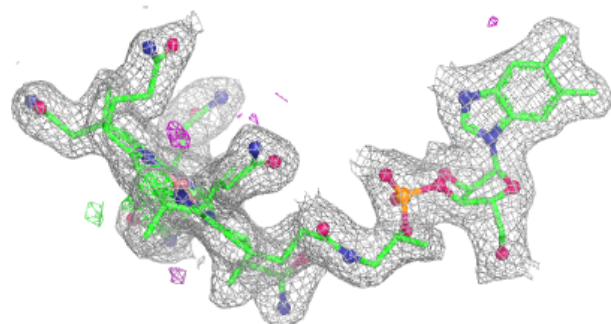
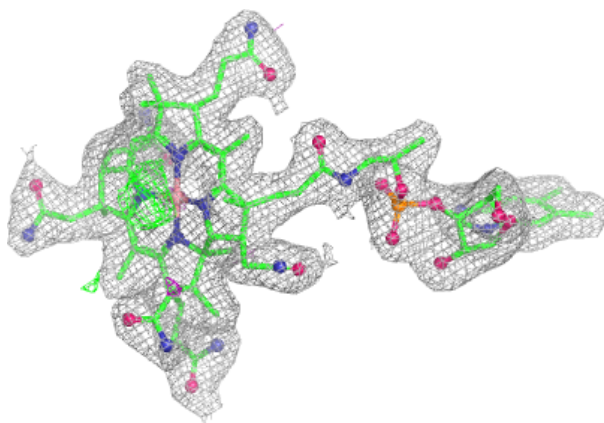


Electron density around SCA C 801 (A):

$2mF_o-DF_c$ (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.