



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:44 AM EDT

PDB ID : 1REQ / pdb_00001req
Title : METHYLMALONYL-COA MUTASE
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1996-01-19
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

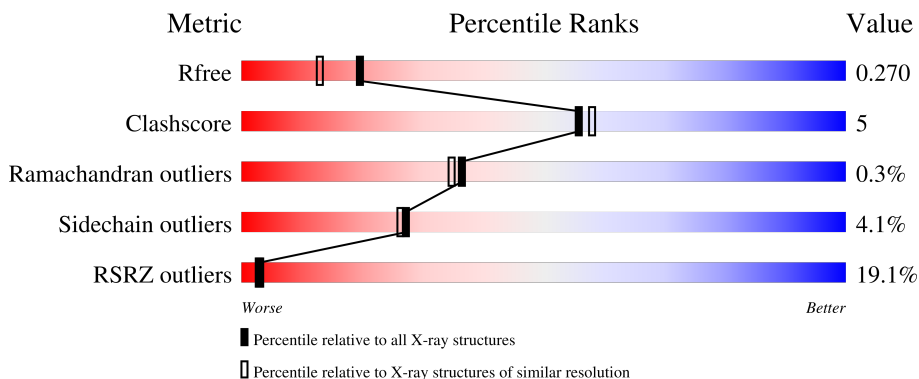
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 12% 53% 41% 5%
1	C	727	 11% 50% 39% 9%
2	B	637	 16% 53% 36% 8%
2	D	637	 39% 54% 35% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22372 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	727	5563	3514	960	1065	24	0	0	0
1	C	727	5560	3515	960	1061	24	0	0	0

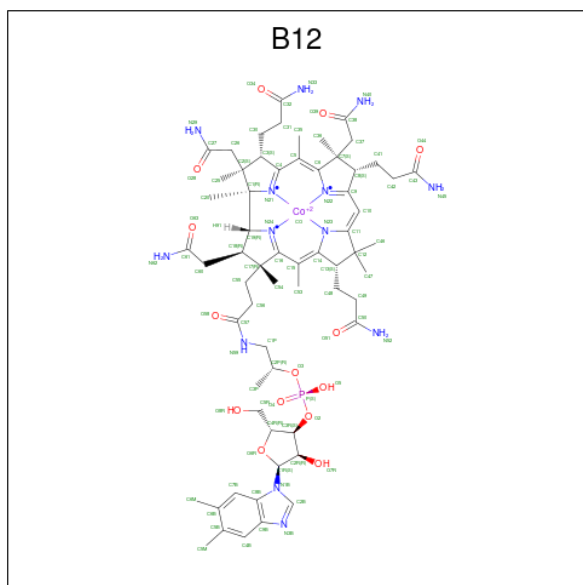
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	4695	2962	820	900	13	0	0	0
2	D	622	4692	2958	818	903	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

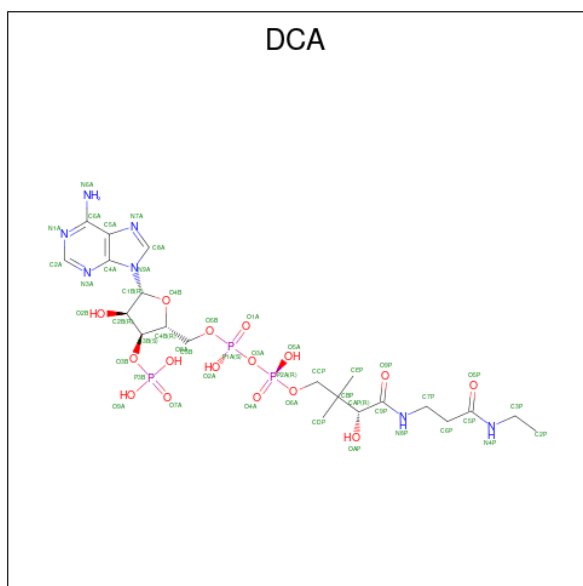
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	conflict	UNP P11652
B	330	GLU	ASP	conflict	UNP P11652
B	331	LEU	VAL	conflict	UNP P11652
D	203	GLY	ALA	conflict	UNP P11652
D	330	GLU	ASP	conflict	UNP P11652
D	331	LEU	VAL	conflict	UNP P11652

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



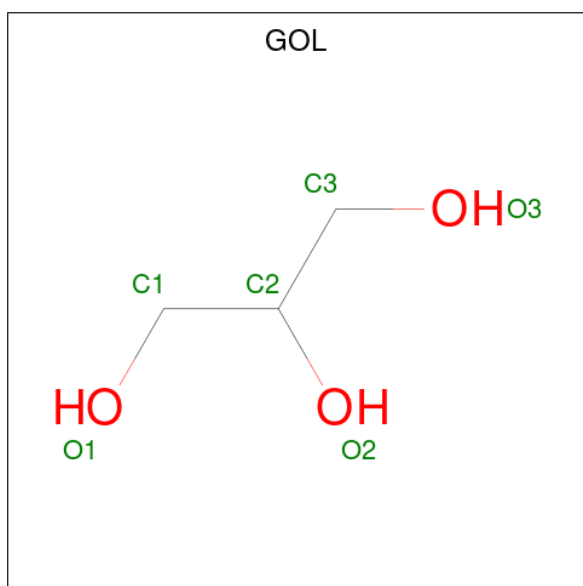
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
3	A	1	91	62	1	13	14	1	0	0
3	C	1	91	62	1	13	14	1	0	0

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	457	Total O 457 457	0	0
6	B	318	Total O 318 318	0	0

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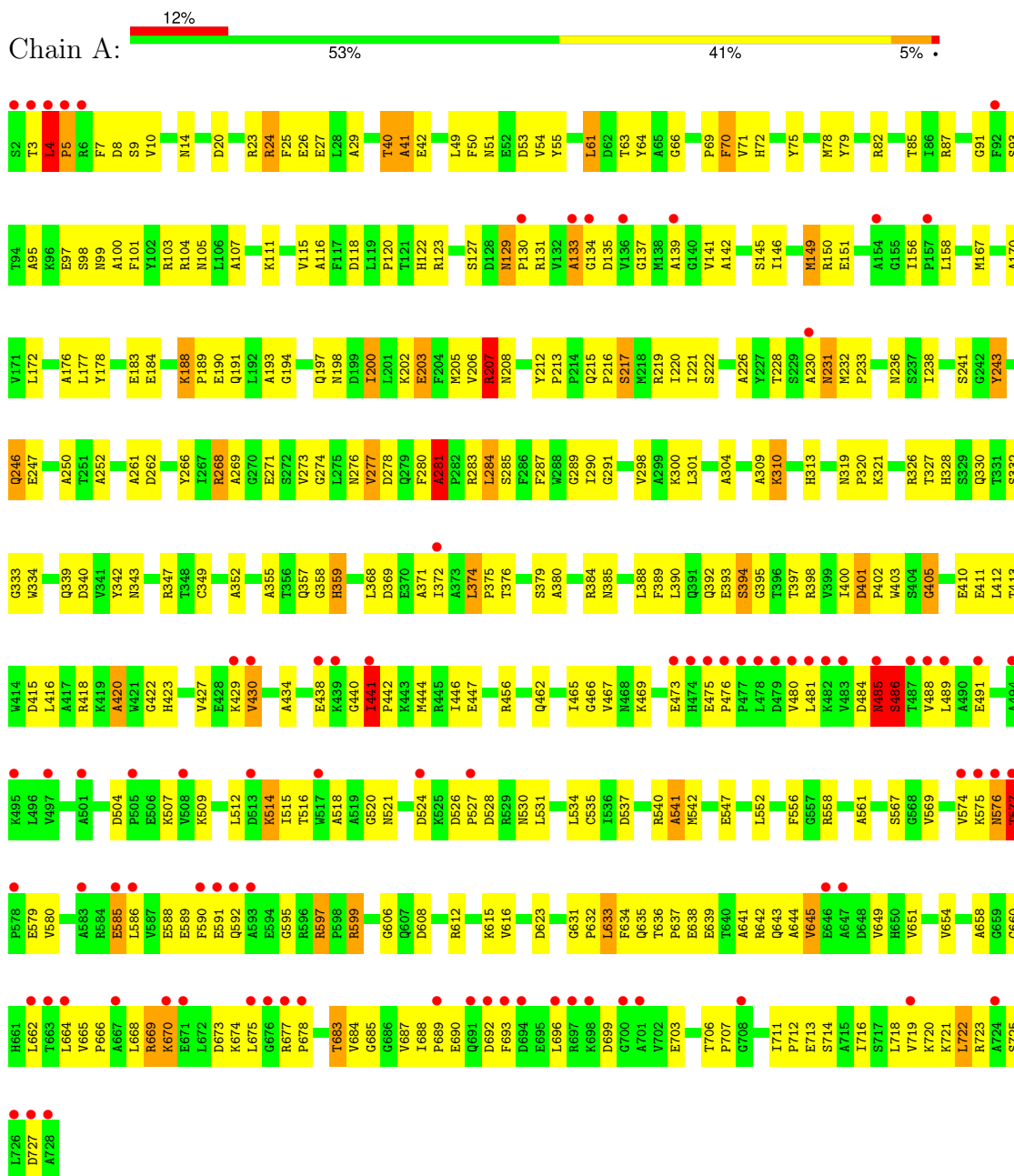
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	493	Total 493	O 493	0	0
6	D	264	Total 264	O 264	0	0

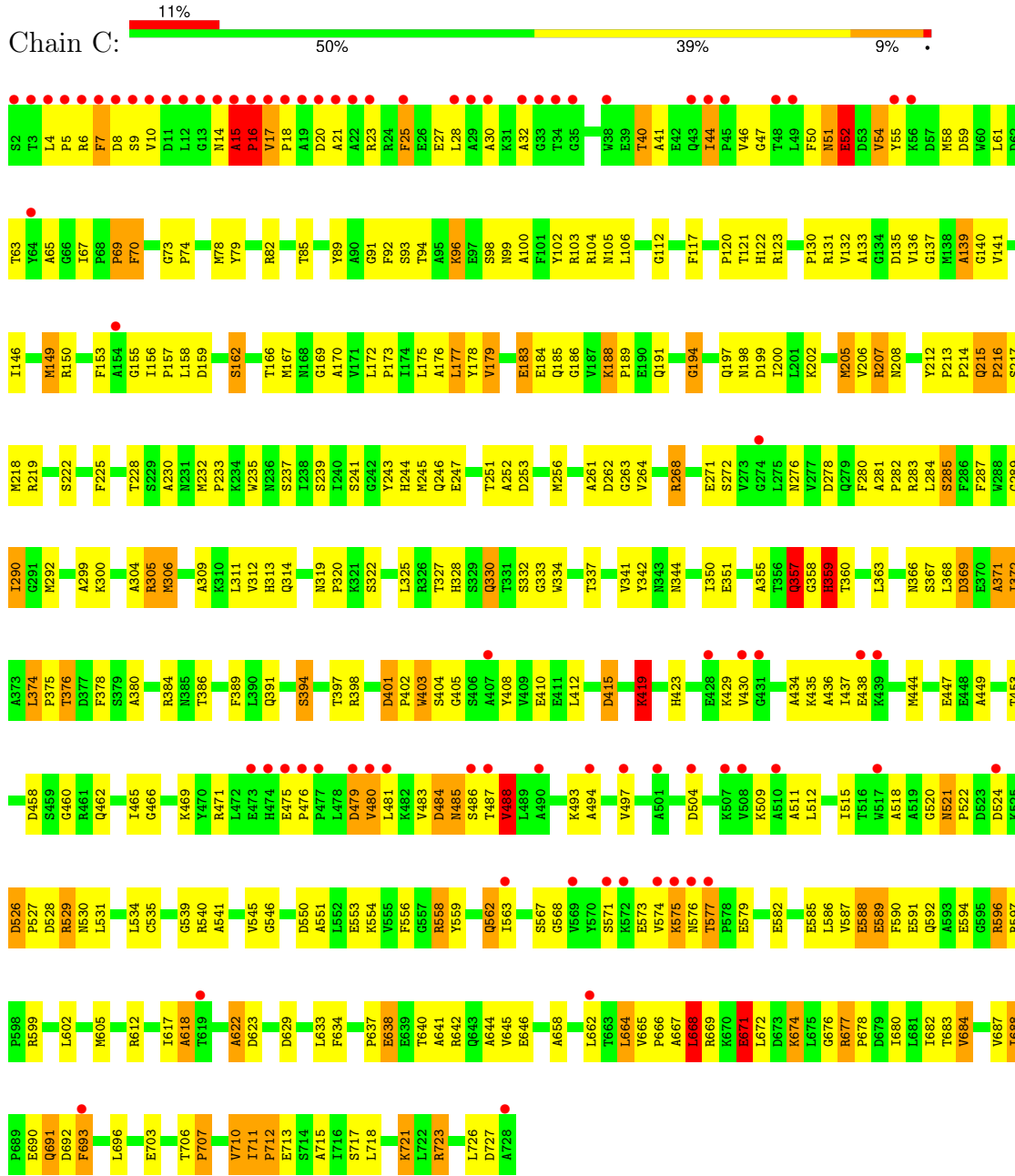
3 Residue-property plots i

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.

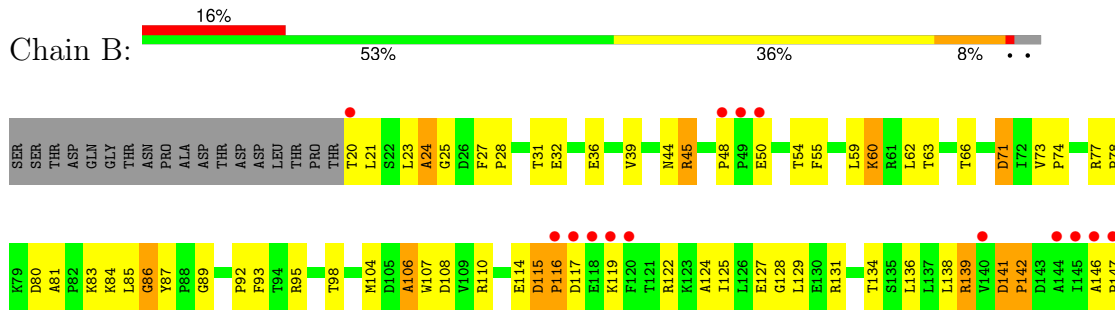
• Molecule 1: METHYLMALONYL-COA MUTASE

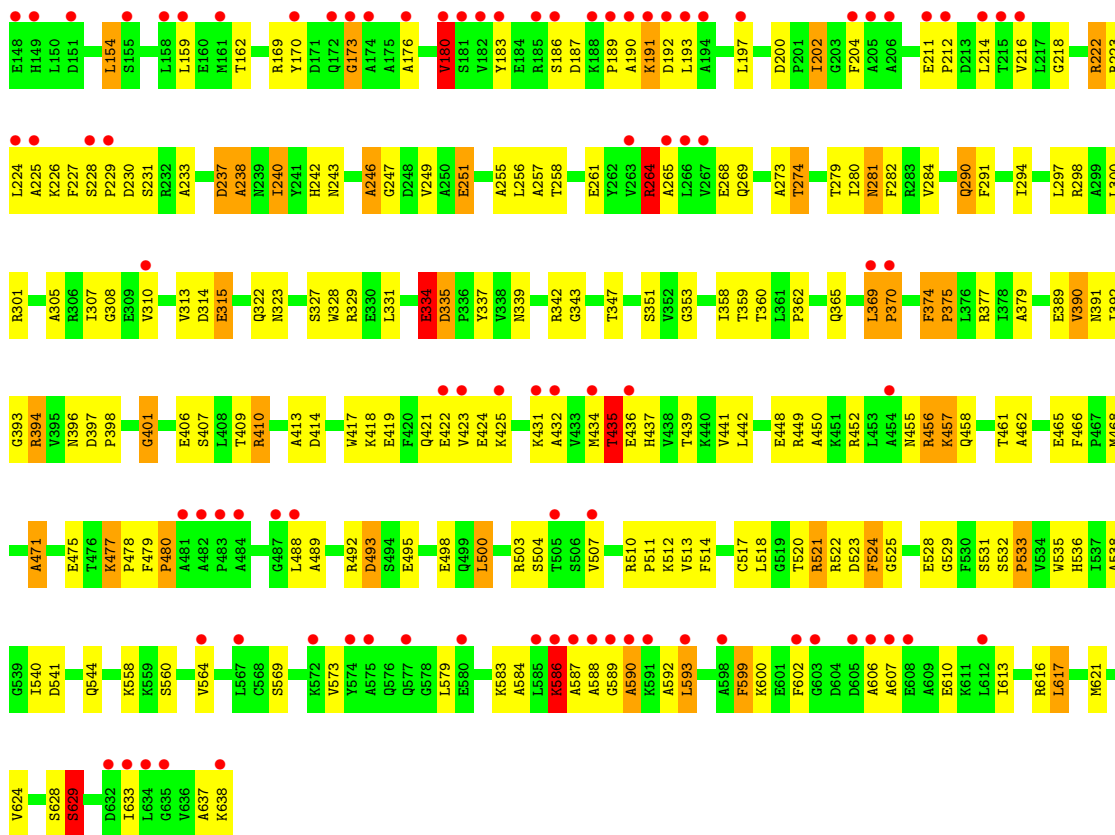


● Molecule 1: METHYLMALONYL-COA MUTASE

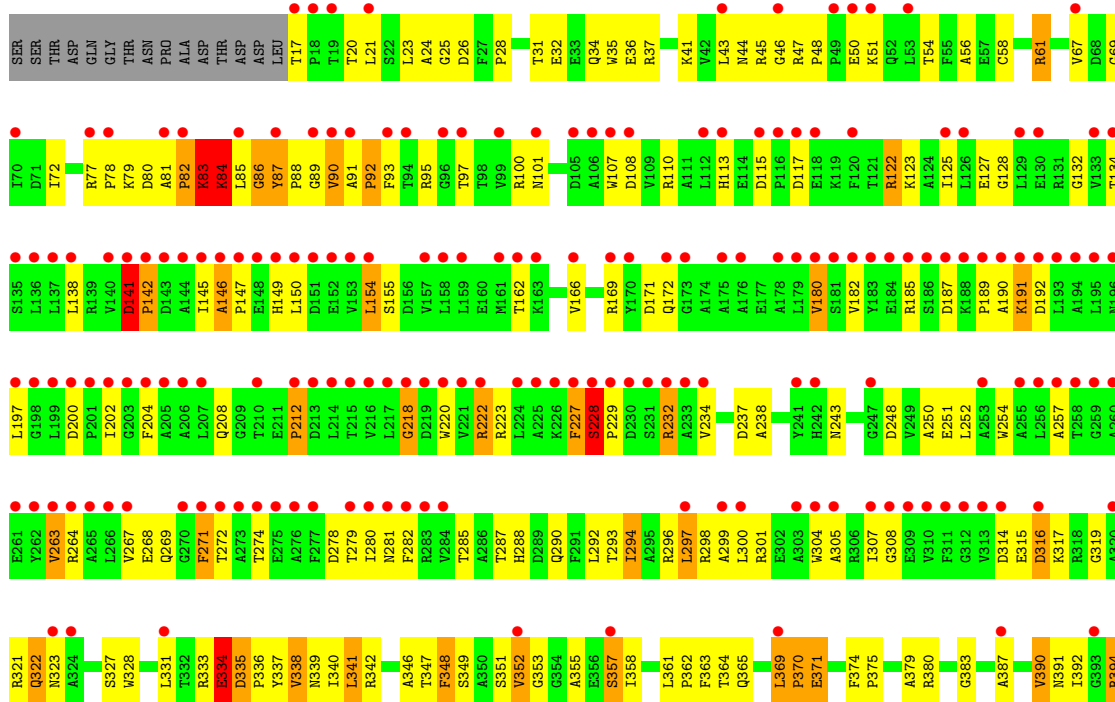
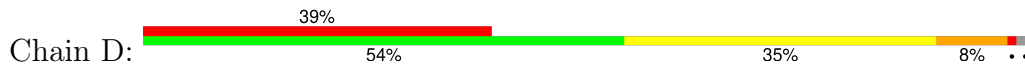


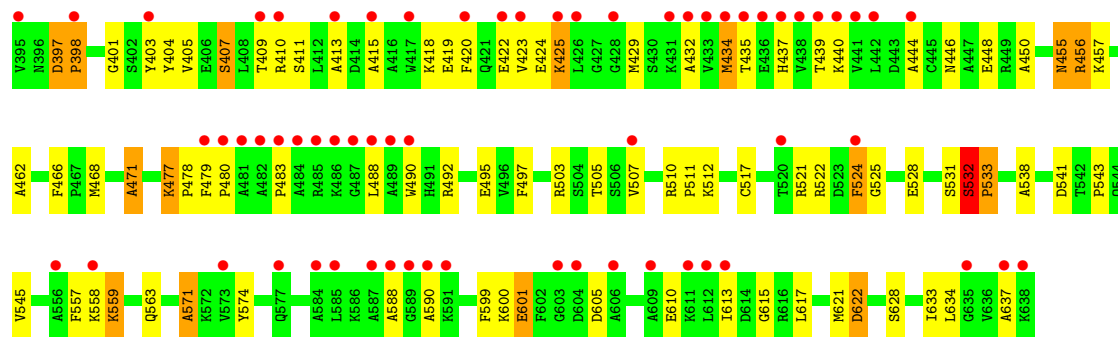
● Molecule 2: METHYLMALONYL-COA MUTASE





● 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	119.80Å 161.30Å 88.40Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.28 (at 1.98Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.275 0.250 , 0.270	Depositor DCC
R_{free} test set	10942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtrriage
Anisotropy	0.568	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.22	5/5679 (0.1%)	2.63	495/7718 (6.4%)
1	C	1.30	8/5676 (0.1%)	2.66	539/7711 (7.0%)
2	B	1.12	8/4785 (0.2%)	2.56	405/6499 (6.2%)
2	D	0.99	1/4783 (0.0%)	2.61	399/6503 (6.1%)
All	All	1.17	22/20923 (0.1%)	2.62	1838/28431 (6.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	C	0	37
2	B	0	21
2	D	0	17
All	All	0	100

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	PHE	CA-CB	8.06	1.59	1.52
2	B	466	PHE	CA-CB	6.68	1.58	1.52
1	C	122	HIS	N-CA	-6.36	1.38	1.46
1	C	300	LYS	CA-C	-6.09	1.44	1.52
1	A	72	HIS	CE1-NE2	-6.01	1.26	1.32
1	C	558	ARG	NE-CZ	5.95	1.39	1.33
1	C	141	VAL	CA-C	5.86	1.59	1.52
2	B	87	TYR	CA-CB	5.71	1.63	1.54
2	B	397	ASP	CA-CB	5.65	1.57	1.52
1	C	684	VAL	C-O	-5.62	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	466	PHE	CA-C	-5.52	1.48	1.53
2	B	458	GLN	N-CA	-5.38	1.40	1.46
1	C	668	LEU	N-CA	-5.34	1.40	1.46
1	A	172	LEU	CA-C	-5.29	1.46	1.52
1	C	91	GLY	N-CA	5.28	1.53	1.45
1	A	85	THR	CA-CB	5.16	1.60	1.53
1	A	238	ILE	CA-C	5.12	1.58	1.52
2	B	406	GLU	C-O	-5.10	1.18	1.24
2	B	531	SER	CA-C	-5.09	1.46	1.52
2	B	535	TRP	CA-CB	5.09	1.61	1.53
1	C	512	LEU	C-N	5.03	1.41	1.34
1	A	222	SER	CA-C	-5.02	1.45	1.52

All (1838) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	264	ARG	CD-NE-CZ	38.39	178.14	124.40
2	D	169	ARG	CD-NE-CZ	29.83	166.16	124.40
1	C	384	ARG	CD-NE-CZ	24.97	159.35	124.40
1	A	384	ARG	CD-NE-CZ	24.42	158.59	124.40
1	C	596	ARG	CD-NE-CZ	19.42	151.59	124.40
1	C	485	ASN	CA-CB-CG	18.86	131.46	112.60
1	A	485	ASN	CA-CB-CG	17.71	130.31	112.60
1	A	485	ASN	N-CA-CB	15.93	133.11	110.01
1	A	23	ARG	CD-NE-CZ	15.52	146.13	124.40
1	C	215	GLN	CA-C-O	15.42	133.59	118.79
2	B	86	GLY	O-C-N	-15.31	106.52	122.60
1	C	664	LEU	CA-C-N	14.51	131.94	120.33
1	C	664	LEU	C-N-CA	14.51	131.94	120.33
2	B	457	LYS	CA-C-N	13.87	140.22	123.16
2	B	457	LYS	C-N-CA	13.87	140.22	123.16
1	A	684	VAL	CA-C-N	-13.72	110.30	121.82
1	A	684	VAL	C-N-CA	-13.72	110.30	121.82
1	C	215	GLN	O-C-N	-13.42	109.78	120.38
1	A	530	ASN	OD1-CG-ND2	13.20	135.80	122.60
2	B	77	ARG	CD-NE-CZ	13.02	142.63	124.40
2	D	507	VAL	CA-C-N	12.40	136.90	120.28
2	D	507	VAL	C-N-CA	12.40	136.90	120.28
2	D	333	ARG	NE-CZ-NH2	12.15	130.14	119.20
1	C	82	ARG	CD-NE-CZ	11.92	141.09	124.40
1	A	103	ARG	CD-NE-CZ	11.84	140.98	124.40
1	A	526	ASP	CA-CB-CG	11.69	124.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	353	GLY	CA-C-N	11.68	140.85	121.00
2	D	353	GLY	C-N-CA	11.68	140.85	121.00
1	C	333	GLY	O-C-N	-11.66	110.99	122.19
1	A	576	ASN	CA-CB-CG	11.50	124.10	112.60
2	B	89	GLY	CA-C-N	11.49	139.41	122.75
2	B	89	GLY	C-N-CA	11.49	139.41	122.75
1	C	103	ARG	CD-NE-CZ	11.47	140.46	124.40
2	D	147	PRO	CA-C-N	11.42	135.96	120.54
2	D	147	PRO	C-N-CA	11.42	135.96	120.54
1	C	430	VAL	O-C-N	-11.29	108.45	122.57
2	B	169	ARG	CD-NE-CZ	10.91	139.68	124.40
2	D	192	ASP	CA-CB-CG	10.91	123.51	112.60
1	C	8	ASP	CA-CB-CG	10.88	123.48	112.60
2	D	117	ASP	CA-CB-CG	10.75	123.35	112.60
1	A	520	GLY	O-C-N	-10.59	110.73	122.28
1	A	238	ILE	O-C-N	10.58	132.18	122.97
1	C	597	ARG	CD-NE-CZ	10.54	139.15	124.40
2	B	466	PHE	O-C-N	-10.52	116.69	121.53
1	A	207	ARG	CB-CG-CD	10.52	135.48	111.30
1	C	213	PRO	CA-C-N	10.50	130.16	119.24
1	C	213	PRO	C-N-CA	10.50	130.16	119.24
2	D	322	GLN	CA-C-O	10.35	131.54	120.36
1	A	690	GLU	CA-C-N	10.35	134.56	120.38
1	A	690	GLU	C-N-CA	10.35	134.56	120.38
2	D	191	LYS	CA-C-N	10.30	134.45	120.44
2	D	191	LYS	C-N-CA	10.30	134.45	120.44
2	D	86	GLY	O-C-N	-10.29	110.84	122.68
1	A	485	ASN	CB-CA-C	-10.17	94.92	110.88
2	B	95	ARG	NE-CZ-NH2	-10.09	110.11	119.20
1	A	727	ASP	CA-CB-CG	10.08	122.68	112.60
1	A	476	PRO	N-CA-CB	10.03	108.80	103.19
2	B	410	ARG	CD-NE-CZ	9.99	138.39	124.40
2	D	314	ASP	CA-CB-CG	9.97	122.57	112.60
1	A	662	LEU	CA-C-O	-9.95	109.89	120.63
2	B	558	LYS	O-C-N	-9.91	111.61	122.12
1	A	485	ASN	OD1-CG-ND2	9.88	132.49	122.60
1	A	298	VAL	O-C-N	-9.85	112.26	121.91
2	B	255	ALA	CA-C-N	9.83	133.22	120.44
2	B	255	ALA	C-N-CA	9.83	133.22	120.44
2	B	77	ARG	NE-CZ-NH2	-9.82	110.36	119.20
1	A	333	GLY	O-C-N	-9.78	112.79	122.18
1	A	526	ASP	CA-C-O	9.74	128.90	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	SER	O-C-N	-9.74	110.29	122.27
1	C	183	GLU	O-C-N	-9.74	111.80	122.12
1	C	313	HIS	CA-C-N	9.72	134.28	120.28
1	C	313	HIS	C-N-CA	9.72	134.28	120.28
2	B	536	HIS	CA-C-N	9.68	133.08	120.60
2	B	536	HIS	C-N-CA	9.68	133.08	120.60
2	D	307	ILE	CA-C-N	9.65	130.84	120.03
2	D	307	ILE	C-N-CA	9.65	130.84	120.03
1	C	535	CYS	O-C-N	-9.63	111.91	122.12
2	D	93	PHE	CA-C-N	9.57	133.46	120.54
2	D	93	PHE	C-N-CA	9.57	133.46	120.54
1	C	711	ILE	CA-C-O	9.54	125.08	118.69
1	A	183	GLU	O-C-N	-9.50	112.05	122.12
2	B	222	ARG	CD-NE-CZ	9.47	137.66	124.40
2	B	422	GLU	O-C-N	-9.47	112.09	122.12
1	C	17	VAL	N-CA-CB	9.45	124.44	111.21
1	A	633	LEU	O-C-N	-9.40	111.59	122.68
1	C	723	ARG	NE-CZ-NH1	9.40	130.90	121.50
2	B	187	ASP	CA-CB-CG	9.36	121.96	112.60
1	A	100	ALA	CA-C-O	-9.35	111.07	120.70
2	B	89	GLY	O-C-N	-9.34	110.74	122.41
2	B	25	GLY	O-C-N	-9.25	112.11	122.84
1	A	268	ARG	NE-CZ-NH2	-9.23	110.90	119.20
2	D	337	TYR	CA-C-N	9.19	134.98	120.47
2	D	337	TYR	C-N-CA	9.19	134.98	120.47
1	C	727	ASP	CA-C-N	9.16	138.19	121.70
1	C	727	ASP	C-N-CA	9.16	138.19	121.70
2	B	600	LYS	CA-C-N	9.14	135.23	120.60
2	B	600	LYS	C-N-CA	9.14	135.23	120.60
2	D	238	ALA	CA-C-N	9.13	133.42	120.28
2	D	238	ALA	C-N-CA	9.13	133.42	120.28
1	C	530	ASN	OD1-CG-ND2	9.12	131.72	122.60
1	C	41	ALA	O-C-N	-9.11	110.54	122.39
2	D	44	ASN	OD1-CG-ND2	9.11	131.71	122.60
1	A	488	VAL	N-CA-CB	9.11	122.23	110.57
2	B	78	PRO	O-C-N	-9.10	111.78	122.24
1	C	412	LEU	CA-C-N	9.08	132.63	120.65
1	C	412	LEU	C-N-CA	9.08	132.63	120.65
2	D	599	PHE	CA-C-N	9.06	133.61	120.38
2	D	599	PHE	C-N-CA	9.06	133.61	120.38
1	A	535	CYS	O-C-N	-9.03	111.85	122.15
2	D	321	ARG	NE-CZ-NH2	-9.04	111.07	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	TYR	CA-C-O	9.01	130.78	120.96
1	C	61	LEU	O-C-N	-9.01	110.61	122.59
1	C	198	ASN	O-C-N	-8.99	111.40	122.55
1	C	691	GLN	OE1-CD-NE2	8.98	131.58	122.60
1	A	547	GLU	CA-C-O	8.97	130.24	120.82
2	D	308	GLY	CA-C-N	8.94	132.26	120.28
2	D	308	GLY	C-N-CA	8.94	132.26	120.28
2	B	85	LEU	CA-C-N	-8.94	110.77	121.85
2	B	85	LEU	C-N-CA	-8.94	110.77	121.85
1	A	226	ALA	O-C-N	-8.94	112.65	122.12
2	B	268	GLU	CA-C-O	-8.89	111.13	120.55
2	B	87	TYR	CA-C-O	8.88	129.62	120.03
2	D	528	GLU	CA-C-N	8.86	129.81	119.98
2	D	528	GLU	C-N-CA	8.86	129.81	119.98
2	D	541	ASP	O-C-N	-8.83	112.72	122.79
1	C	313	HIS	O-C-N	-8.82	112.14	122.20
2	B	461	THR	CA-C-O	8.79	130.54	120.96
1	C	332	SER	O-C-N	-8.78	111.40	122.82
2	B	282	PHE	CA-CB-CG	8.76	122.56	113.80
1	C	378	PHE	O-C-N	-8.75	113.06	122.07
1	A	641	ALA	CA-C-N	8.74	132.00	120.28
1	A	641	ALA	C-N-CA	8.74	132.00	120.28
1	C	139	ALA	CA-C-N	8.72	132.95	120.91
1	C	139	ALA	C-N-CA	8.72	132.95	120.91
2	D	110	ARG	CD-NE-CZ	8.72	136.61	124.40
1	A	78	MET	O-C-N	-8.71	111.01	122.59
1	A	228	THR	O-C-N	-8.71	111.56	122.27
1	C	332	SER	CA-C-O	8.69	130.42	120.60
1	C	136	VAL	N-CA-CB	8.69	120.46	110.82
2	D	141	ASP	CA-CB-CG	8.66	121.27	112.60
2	D	369	LEU	CA-C-O	8.66	128.40	120.60
1	C	485	ASN	CB-CA-C	-8.66	97.16	110.92
2	B	147	PRO	CA-C-N	8.65	135.17	120.72
2	B	147	PRO	C-N-CA	8.65	135.17	120.72
1	A	146	ILE	CA-C-N	8.65	132.22	120.54
1	A	146	ILE	C-N-CA	8.65	132.22	120.54
2	D	24	ALA	CA-C-N	8.64	129.71	120.03
2	D	24	ALA	C-N-CA	8.64	129.71	120.03
2	D	269	GLN	CA-C-N	8.64	134.64	121.51
2	D	269	GLN	C-N-CA	8.64	134.64	121.51
1	C	633	LEU	CA-C-N	8.63	136.67	123.47
1	C	633	LEU	C-N-CA	8.63	136.67	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	639	GLU	CA-C-N	8.62	131.64	120.44
1	A	639	GLU	C-N-CA	8.62	131.64	120.44
2	B	339	ASN	O-C-N	-8.58	112.18	122.22
1	C	333	GLY	CA-C-N	8.58	132.13	120.38
1	C	333	GLY	C-N-CA	8.58	132.13	120.38
1	A	41	ALA	O-C-N	-8.57	110.94	122.43
2	B	337	TYR	O-C-N	-8.57	111.25	122.39
1	C	465	ILE	CA-C-O	8.54	131.04	121.13
1	C	309	ALA	CA-C-O	-8.53	111.86	120.82
2	D	315	GLU	CA-C-N	8.53	137.82	122.38
2	D	315	GLU	C-N-CA	8.53	137.82	122.38
1	A	678	PRO	CA-C-O	8.53	128.01	118.38
1	C	263	GLY	O-C-N	-8.52	114.01	122.19
1	C	488	VAL	N-CA-CB	8.51	119.89	110.62
1	C	300	LYS	O-C-N	-8.50	113.25	122.09
1	C	545	VAL	O-C-N	-8.50	113.58	121.91
1	A	111	LYS	CA-C-N	-8.48	116.33	122.18
1	A	111	LYS	C-N-CA	-8.48	116.33	122.18
1	A	488	VAL	CB-CA-C	-8.48	100.91	112.02
1	A	287	PHE	CA-CB-CG	8.47	122.28	113.80
2	D	339	ASN	O-C-N	-8.47	111.37	122.39
2	B	422	GLU	CA-CB-CG	8.46	131.03	114.10
1	A	145	SER	CA-C-N	8.46	132.05	120.46
1	A	145	SER	C-N-CA	8.46	132.05	120.46
1	A	693	PHE	CA-CB-CG	8.46	122.26	113.80
1	A	375	PRO	N-CA-CB	8.46	110.71	103.35
1	A	418	ARG	CA-C-O	-8.46	111.99	120.70
1	A	188	LYS	CA-C-N	8.42	128.54	119.28
1	A	188	LYS	C-N-CA	8.42	128.54	119.28
2	D	541	ASP	CA-C-O	8.42	131.63	121.87
1	A	575	LYS	CA-C-N	8.37	134.04	122.07
1	A	575	LYS	C-N-CA	8.37	134.04	122.07
1	A	597	ARG	CD-NE-CZ	8.37	136.11	124.40
1	C	677	ARG	NE-CZ-NH2	8.37	126.73	119.20
1	A	333	GLY	CA-C-O	8.35	130.01	121.00
2	B	410	ARG	NE-CZ-NH2	-8.34	111.69	119.20
1	A	135	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	71	VAL	O-C-N	-8.34	113.25	121.83
2	D	466	PHE	O-C-N	-8.32	117.70	121.53
1	A	66	GLY	O-C-N	-8.31	112.20	122.34
2	D	466	PHE	CA-C-O	8.31	126.91	120.26
1	C	378	PHE	CA-C-N	8.30	131.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	PHE	C-N-CA	8.30	131.40	120.28
2	D	72	ILE	CB-CG1-CD1	8.29	131.22	113.80
1	C	322	SER	O-C-N	-8.28	113.34	122.12
1	C	122	HIS	CA-CB-CG	-8.27	105.53	113.80
2	D	95	ARG	CG-CD-NE	8.27	130.19	112.00
2	B	60	LYS	O-C-N	-8.26	113.36	122.12
2	D	425	LYS	CA-C-N	8.26	136.17	122.54
2	D	425	LYS	C-N-CA	8.26	136.17	122.54
1	A	232	MET	O-C-N	-8.26	113.94	121.37
1	C	146	ILE	O-C-N	-8.26	113.56	121.90
2	D	524	PHE	CA-CB-CG	8.25	122.05	113.80
2	B	599	PHE	O-C-N	-8.23	112.59	122.22
1	C	360	THR	O-C-N	-8.23	113.41	122.79
2	D	84	LYS	CB-CG-CD	8.19	130.13	111.30
2	D	349	SER	CA-C-N	8.19	131.92	120.29
2	D	349	SER	C-N-CA	8.19	131.92	120.29
1	C	131	ARG	CD-NE-CZ	8.18	135.85	124.40
1	C	368	LEU	O-C-N	-8.17	112.66	122.22
2	D	263	VAL	N-CA-C	-8.17	102.74	110.42
1	A	217	SER	CA-C-N	8.15	131.20	120.28
1	A	217	SER	C-N-CA	8.15	131.20	120.28
1	A	313	HIS	CA-C-N	8.14	132.26	120.38
1	A	313	HIS	C-N-CA	8.14	132.26	120.38
2	D	47	ARG	CA-C-O	8.14	127.94	119.80
2	B	390	VAL	O-C-N	-8.14	110.89	122.12
2	D	407	SER	O-C-N	-8.13	113.38	122.08
2	B	93	PHE	CA-C-N	8.13	131.51	120.54
2	B	93	PHE	C-N-CA	8.13	131.51	120.54
2	B	419	GLU	CA-C-N	8.13	131.00	120.44
2	B	419	GLU	C-N-CA	8.13	131.00	120.44
1	C	545	VAL	CA-C-N	8.11	129.16	119.99
1	C	545	VAL	C-N-CA	8.11	129.16	119.99
2	D	169	ARG	NE-CZ-NH2	8.09	126.48	119.20
2	D	328	TRP	CA-C-O	8.08	129.86	120.00
1	C	612	ARG	CA-C-N	8.07	128.90	119.94
1	C	612	ARG	C-N-CA	8.07	128.90	119.94
2	D	456	ARG	O-C-N	-8.07	111.60	122.41
1	C	423	HIS	CA-CB-CG	8.06	121.86	113.80
1	C	15	ALA	CA-C-N	8.06	129.91	119.84
1	C	15	ALA	C-N-CA	8.06	129.91	119.84
1	C	520	GLY	O-C-N	-8.05	113.58	122.68
1	A	368	LEU	O-C-N	-8.05	112.80	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	GLU	CA-C-N	8.05	131.06	120.28
1	A	591	GLU	C-N-CA	8.05	131.06	120.28
2	D	339	ASN	CA-C-N	8.05	130.70	120.56
2	D	339	ASN	C-N-CA	8.05	130.70	120.56
1	C	592	GLN	OE1-CD-NE2	8.04	130.65	122.60
2	B	28	PRO	N-CA-CB	8.03	110.34	103.35
2	D	305	ALA	CA-C-N	8.01	131.01	120.28
2	D	305	ALA	C-N-CA	8.01	131.01	120.28
2	B	523	ASP	CA-C-O	-8.00	111.99	120.55
1	C	551	ALA	O-C-N	-7.97	113.80	122.09
2	B	390	VAL	CA-C-O	7.97	129.23	119.58
1	C	105	ASN	CA-CB-CG	-7.97	104.63	112.60
2	B	529	GLY	CA-C-N	7.97	131.28	120.44
2	B	529	GLY	C-N-CA	7.97	131.28	120.44
2	B	457	LYS	O-C-N	-7.96	111.11	122.41
1	A	485	ASN	CA-C-O	-7.95	112.48	120.82
2	B	500	LEU	O-C-N	-7.94	113.70	122.12
2	B	450	ALA	CA-C-N	7.94	131.23	120.44
2	B	450	ALA	C-N-CA	7.94	131.23	120.44
1	C	494	ALA	O-C-N	-7.92	113.73	122.12
2	B	95	ARG	NH1-CZ-NH2	7.91	129.59	119.30
1	A	304	ALA	O-C-N	-7.90	113.75	122.12
1	A	664	LEU	N-CA-C	7.89	119.51	111.07
1	A	608	ASP	CA-CB-CG	7.88	120.48	112.60
2	D	462	ALA	O-C-N	-7.88	112.03	121.97
2	B	339	ASN	CA-C-N	7.88	130.77	120.60
2	B	339	ASN	C-N-CA	7.88	130.77	120.60
2	B	95	ARG	CG-CD-NE	7.88	129.33	112.00
1	C	334	TRP	CA-C-N	7.87	133.19	120.60
1	C	334	TRP	C-N-CA	7.87	133.19	120.60
2	D	89	GLY	CA-C-N	7.87	133.99	121.95
2	D	89	GLY	C-N-CA	7.87	133.99	121.95
2	B	558	LYS	CA-C-N	7.86	132.26	120.31
2	B	558	LYS	C-N-CA	7.86	132.26	120.31
2	D	232	ARG	CD-NE-CZ	7.85	135.39	124.40
1	A	178	TYR	O-C-N	-7.85	113.99	122.07
2	B	180	VAL	N-CA-CB	7.83	121.19	110.54
1	A	597	ARG	NE-CZ-NH1	7.82	129.32	121.50
2	D	83	LYS	CA-C-N	7.82	133.17	122.77
2	D	83	LYS	C-N-CA	7.82	133.17	122.77
1	C	357	GLN	O-C-N	-7.82	111.02	122.43
1	C	429	LYS	O-C-N	-7.81	114.03	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ASP	CA-CB-CG	7.79	120.39	112.60
2	B	77	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	C	225	PHE	CA-CB-CG	7.79	121.59	113.80
2	B	281	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	205	MET	CA-C-O	-7.78	112.68	120.70
1	A	690	GLU	O-C-N	-7.77	113.13	122.22
2	B	531	SER	N-CA-C	7.77	121.25	111.69
2	D	45	ARG	CA-C-O	-7.77	112.53	121.07
2	D	296	ARG	CA-C-O	-7.75	112.68	120.82
1	A	429	LYS	CA-C-N	7.72	134.88	122.76
1	A	429	LYS	C-N-CA	7.72	134.88	122.76
2	B	147	PRO	O-C-N	-7.72	112.83	122.17
2	B	435	THR	CA-CB-CG2	7.71	123.62	110.50
1	C	553	GLU	CA-C-N	7.71	130.94	120.38
1	C	553	GLU	C-N-CA	7.71	130.94	120.38
2	B	218	GLY	O-C-N	-7.70	114.50	122.13
2	B	159	LEU	CA-C-N	7.70	133.77	120.68
2	B	159	LEU	C-N-CA	7.70	133.77	120.68
2	D	223	ARG	CA-C-N	7.70	136.42	121.18
2	D	223	ARG	C-N-CA	7.70	136.42	121.18
2	D	420	PHE	CA-CB-CG	7.68	121.48	113.80
2	D	218	GLY	CA-C-N	7.68	130.91	120.54
2	D	218	GLY	C-N-CA	7.68	130.91	120.54
1	C	344	ASN	CA-C-N	7.66	130.22	120.56
1	C	344	ASN	C-N-CA	7.66	130.22	120.56
1	A	54	VAL	CA-C-O	-7.66	112.37	120.57
2	D	77	ARG	CA-C-O	7.66	130.66	120.16
2	B	410	ARG	NE-CZ-NH1	7.66	129.16	121.50
2	D	390	VAL	CA-C-O	7.65	127.99	119.42
1	C	589	GLU	O-C-N	-7.63	114.03	122.12
2	D	294	ILE	CA-C-N	7.61	130.81	120.54
2	D	294	ILE	C-N-CA	7.61	130.81	120.54
1	C	550	ASP	CA-CB-CG	7.59	120.19	112.60
2	D	390	VAL	O-C-N	-7.59	113.23	122.18
1	A	129	ASN	CA-C-N	7.58	127.62	119.28
1	A	129	ASN	C-N-CA	7.58	127.62	119.28
1	C	120	PRO	O-C-N	-7.58	113.99	122.18
1	A	100	ALA	N-CA-C	-7.57	102.97	111.14
2	D	69	GLY	N-CA-C	7.55	125.50	114.10
1	C	285	SER	O-C-N	-7.54	114.05	123.17
2	D	162	THR	N-CA-C	7.53	121.20	109.07
1	C	92	PHE	CA-CB-CG	-7.53	106.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	316	ASP	CA-CB-CG	7.53	120.13	112.60
1	C	357	GLN	CA-C-O	7.53	128.75	119.11
1	A	146	ILE	O-C-N	-7.51	114.58	121.87
1	A	456	ARG	CD-NE-CZ	7.51	134.91	124.40
2	B	77	ARG	O-C-N	-7.50	114.94	121.32
1	C	577	THR	CA-C-O	7.50	126.49	120.19
1	A	327	THR	N-CA-C	7.50	120.85	109.23
2	D	132	GLY	N-CA-C	7.50	125.30	115.40
1	C	78	MET	O-C-N	-7.50	112.62	122.59
2	D	521	ARG	O-C-N	-7.50	114.17	122.12
1	A	232	MET	CA-C-N	7.49	127.13	119.56
1	A	232	MET	C-N-CA	7.49	127.13	119.56
1	A	170	ALA	CA-C-N	7.49	131.05	120.42
1	A	170	ALA	C-N-CA	7.49	131.05	120.42
2	B	242	HIS	O-C-N	-7.47	114.32	122.09
1	C	222	SER	O-C-N	-7.47	114.20	122.12
2	B	600	LYS	O-C-N	-7.47	112.68	122.39
2	D	58	CYS	CA-C-O	7.46	128.33	120.42
1	A	281	ALA	O-C-N	-7.46	112.74	121.32
2	D	88	PRO	N-CA-CB	7.46	110.28	103.19
2	B	124	ALA	O-C-N	-7.43	114.42	122.07
2	D	347	THR	O-C-N	-7.42	114.25	122.12
1	A	313	HIS	O-C-N	-7.41	114.26	122.12
1	A	441	ILE	CA-C-O	7.41	123.66	118.69
1	C	688	ILE	CA-C-O	7.39	129.86	119.95
2	D	23	LEU	O-C-N	-7.39	114.55	121.79
2	B	106	ALA	CA-C-O	-7.39	112.04	120.24
1	A	547	GLU	O-C-N	-7.38	114.47	122.07
1	C	276	ASN	CA-C-N	7.38	130.57	120.46
1	C	276	ASN	C-N-CA	7.38	130.57	120.46
1	C	556	PHE	CA-CB-CG	7.38	121.18	113.80
2	D	558	LYS	CA-C-N	7.38	130.16	120.28
2	D	558	LYS	C-N-CA	7.38	130.16	120.28
1	A	673	ASP	O-C-N	-7.37	114.48	122.07
2	B	573	VAL	CA-C-O	-7.37	113.28	120.95
1	A	369	ASP	CA-C-N	7.37	130.89	120.28
1	A	369	ASP	C-N-CA	7.37	130.89	120.28
1	C	437	ILE	CA-C-O	-7.37	113.61	121.27
1	A	281	ALA	CA-C-N	7.36	127.00	119.56
1	A	281	ALA	C-N-CA	7.36	127.00	119.56
1	A	410	GLU	CB-CG-CD	7.35	125.09	112.60
1	C	79	TYR	CA-C-N	7.34	130.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	TYR	C-N-CA	7.34	130.12	120.28
1	A	332	SER	CA-C-O	7.33	129.08	120.58
2	D	339	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	678	PRO	CA-C-N	7.31	133.10	120.68
1	A	678	PRO	C-N-CA	7.31	133.10	120.68
1	A	319	ASN	CA-CB-CG	7.31	119.91	112.60
2	D	370	PRO	N-CA-CB	7.30	109.45	103.32
2	D	479	PHE	CA-CB-CG	7.30	121.10	113.80
1	A	398	ARG	O-C-N	-7.30	112.65	122.43
1	C	397	THR	O-C-N	-7.30	112.46	122.46
1	A	51	ASN	CA-C-N	7.29	132.27	120.60
1	A	51	ASN	C-N-CA	7.29	132.27	120.60
1	A	434	ALA	CA-C-N	7.28	130.63	120.29
1	A	434	ALA	C-N-CA	7.28	130.63	120.29
2	D	271	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	466	GLY	O-C-N	-7.27	112.89	122.42
2	B	461	THR	CA-CB-OG1	-7.27	98.70	109.60
2	D	418	LYS	CA-C-O	-7.26	112.07	120.20
1	C	312	VAL	N-CA-CB	7.26	121.47	110.58
1	A	137	GLY	CA-C-N	7.25	132.99	120.58
1	A	137	GLY	C-N-CA	7.25	132.99	120.58
2	D	437	HIS	CA-CB-CG	-7.25	106.55	113.80
2	B	301	ARG	CA-C-O	-7.24	112.87	120.55
2	D	533	PRO	N-CA-CB	7.24	111.30	103.33
1	A	673	ASP	CA-C-N	7.24	130.70	120.28
1	A	673	ASP	C-N-CA	7.24	130.70	120.28
2	B	397	ASP	CA-C-N	7.23	126.94	119.56
2	B	397	ASP	C-N-CA	7.23	126.94	119.56
1	C	59	ASP	CA-C-O	-7.22	111.07	119.59
1	C	690	GLU	CA-C-N	7.21	129.94	120.28
1	C	690	GLU	C-N-CA	7.21	129.94	120.28
1	C	527	PRO	N-CA-CB	7.20	111.17	103.39
2	D	169	ARG	NE-CZ-NH1	-7.20	114.30	121.50
2	D	531	SER	N-CA-C	7.19	120.54	111.69
2	D	457	LYS	O-C-N	-7.19	112.20	122.41
1	C	337	THR	CA-C-O	7.19	130.26	121.56
2	B	342	ARG	CD-NE-CZ	-7.19	114.34	124.40
1	C	198	ASN	CA-CB-CG	7.18	119.78	112.60
1	A	115	VAL	N-CA-C	7.18	119.22	108.23
2	D	32	GLU	O-C-N	-7.18	114.62	122.09
2	D	191	LYS	N-CA-C	7.18	121.13	112.38
1	C	281	ALA	O-C-N	-7.17	113.97	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ASN	O-C-N	-7.17	113.83	122.22
2	B	369	LEU	CA-C-O	7.17	126.21	120.19
2	B	261	GLU	O-C-N	-7.17	114.63	122.09
1	A	516	THR	CA-C-N	7.16	129.75	120.44
1	A	516	THR	C-N-CA	7.16	129.75	120.44
1	C	357	GLN	OE1-CD-NE2	-7.16	115.44	122.60
2	B	202	ILE	CA-C-N	7.15	127.91	119.98
2	B	202	ILE	C-N-CA	7.15	127.91	119.98
1	C	410	GLU	CB-CG-CD	7.15	124.75	112.60
1	C	599	ARG	CG-CD-NE	7.14	127.72	112.00
1	A	25	PHE	O-C-N	-7.14	114.38	122.09
2	D	79	LYS	O-C-N	-7.14	114.06	122.20
1	C	232	MET	CA-C-N	7.14	126.77	119.56
1	C	232	MET	C-N-CA	7.14	126.77	119.56
2	D	525	GLY	CA-C-N	7.14	127.86	119.94
2	D	525	GLY	C-N-CA	7.14	127.86	119.94
1	C	149	MET	CA-C-N	7.13	129.84	120.28
1	C	149	MET	C-N-CA	7.13	129.84	120.28
1	C	551	ALA	CA-C-N	7.13	129.84	120.28
1	C	551	ALA	C-N-CA	7.13	129.84	120.28
1	C	178	TYR	O-C-N	-7.13	114.73	122.07
1	A	403	TRP	CA-C-N	7.13	132.60	121.26
1	A	403	TRP	C-N-CA	7.13	132.60	121.26
1	A	692	ASP	CA-C-N	7.12	132.76	120.58
1	A	692	ASP	C-N-CA	7.12	132.76	120.58
2	B	32	GLU	O-C-N	-7.12	114.68	122.09
1	C	410	GLU	CA-C-O	-7.12	113.00	120.55
1	C	344	ASN	O-C-N	-7.12	113.88	122.22
2	D	532	SER	CA-C-N	7.11	126.95	119.05
2	D	532	SER	C-N-CA	7.11	126.95	119.05
1	A	392	GLN	OE1-CD-NE2	-7.11	115.49	122.60
1	C	574	VAL	N-CA-CB	7.11	120.75	112.15
1	C	590	PHE	O-C-N	-7.10	114.76	122.07
2	B	48	PRO	CA-C-N	7.10	128.72	119.84
2	B	48	PRO	C-N-CA	7.10	128.72	119.84
1	A	8	ASP	CA-C-N	7.09	133.74	122.11
1	A	8	ASP	C-N-CA	7.09	133.74	122.11
1	A	712	PRO	CA-C-N	7.09	129.65	120.44
1	A	712	PRO	C-N-CA	7.09	129.65	120.44
1	A	401	ASP	CA-C-N	7.08	126.91	119.05
1	A	401	ASP	C-N-CA	7.08	126.91	119.05
1	A	658	ALA	CA-C-N	7.08	133.74	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	658	ALA	C-N-CA	7.08	133.74	121.07
1	C	52	GLU	CA-C-N	7.08	132.54	120.72
1	C	52	GLU	C-N-CA	7.08	132.54	120.72
1	A	518	ALA	O-C-N	-7.08	114.62	122.12
2	D	423	VAL	CA-C-N	7.07	131.06	120.31
2	D	423	VAL	C-N-CA	7.07	131.06	120.31
2	D	200	ASP	CA-CB-CG	7.07	119.67	112.60
2	D	243	ASN	N-CA-C	7.06	120.79	111.75
2	D	600	LYS	O-C-N	-7.06	114.15	122.20
1	A	658	ALA	O-C-N	-7.06	113.87	122.34
2	B	455	ASN	CA-C-N	7.06	132.14	122.19
2	B	455	ASN	C-N-CA	7.06	132.14	122.19
1	C	268	ARG	NE-CZ-NH2	-7.06	112.85	119.20
2	B	231	SER	CA-C-O	7.06	129.06	121.16
1	C	287	PHE	CA-CB-CG	7.06	120.86	113.80
2	D	182	VAL	CA-C-N	7.06	131.04	120.31
2	D	182	VAL	C-N-CA	7.06	131.04	120.31
1	C	693	PHE	CA-CB-CG	7.06	120.86	113.80
1	C	67	ILE	CA-CB-CG1	7.05	122.39	110.40
1	C	612	ARG	CA-C-O	-7.05	113.36	120.90
2	B	176	ALA	O-C-N	-7.05	114.54	122.08
1	A	118	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	586	LEU	O-C-N	-7.04	113.99	122.22
2	D	446	ASN	CA-C-O	-7.04	112.15	120.10
1	C	212	TYR	O-C-N	-7.03	112.20	121.34
1	C	184	GLU	N-CA-C	7.01	121.28	112.87
2	D	599	PHE	O-C-N	-7.01	114.02	122.22
2	B	32	GLU	CA-C-N	7.00	129.66	120.28
2	B	32	GLU	C-N-CA	7.00	129.66	120.28
2	B	192	ASP	CA-CB-CG	-7.00	105.60	112.60
2	B	590	ALA	CA-C-N	7.00	130.95	120.31
2	B	590	ALA	C-N-CA	7.00	130.95	120.31
2	B	613	ILE	CA-C-O	6.99	128.83	120.65
1	A	75	TYR	O-C-N	-6.98	114.34	123.21
1	C	166	THR	CA-CB-OG1	-6.98	99.13	109.60
2	D	634	LEU	CA-C-N	6.98	135.09	121.41
2	D	634	LEU	C-N-CA	6.98	135.09	121.41
1	C	633	LEU	N-CA-C	-6.97	101.84	110.41
1	C	166	THR	CA-C-O	-6.97	113.78	121.58
1	C	123	ARG	CA-C-N	6.96	133.33	120.87
1	C	123	ARG	C-N-CA	6.96	133.33	120.87
1	A	120	PRO	O-C-N	-6.96	114.31	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ILE	CA-C-O	6.96	129.27	119.95
2	D	77	ARG	O-C-N	-6.95	113.32	121.32
2	D	415	ALA	CA-C-O	-6.95	113.05	120.42
2	B	406	GLU	CB-CG-CD	6.94	124.40	112.60
2	D	48	PRO	CA-C-N	6.94	126.46	119.24
2	D	48	PRO	C-N-CA	6.94	126.46	119.24
1	C	394	SER	CA-C-N	6.94	134.54	120.80
1	C	394	SER	C-N-CA	6.94	134.54	120.80
2	B	200	ASP	CA-CB-CG	6.94	119.54	112.60
2	B	362	PRO	N-CA-CB	6.93	109.38	103.35
1	A	637	PRO	CA-C-N	6.93	132.43	120.58
1	A	637	PRO	C-N-CA	6.93	132.43	120.58
1	C	368	LEU	CA-C-O	6.93	127.93	120.10
1	A	488	VAL	CA-C-N	6.93	130.42	120.79
1	A	488	VAL	C-N-CA	6.93	130.42	120.79
2	B	290	GLN	OE1-CD-NE2	6.93	129.53	122.60
1	A	207	ARG	CA-C-O	6.92	127.37	119.27
2	B	141	ASP	CA-C-O	6.92	126.86	120.56
2	D	557	PHE	CA-C-N	6.92	129.88	120.54
2	D	557	PHE	C-N-CA	6.92	129.88	120.54
2	B	495	GLU	CA-C-O	-6.92	113.16	120.63
2	B	328	TRP	O-C-N	-6.92	113.23	122.23
2	D	51	LYS	N-CA-C	6.92	120.39	109.39
1	A	665	VAL	CA-C-N	6.91	126.38	118.85
1	A	665	VAL	C-N-CA	6.91	126.38	118.85
2	B	191	LYS	N-CA-C	6.90	121.15	112.87
1	C	637	PRO	CA-C-N	6.90	130.09	120.29
1	C	637	PRO	C-N-CA	6.90	130.09	120.29
2	B	141	ASP	CA-C-N	6.90	126.71	119.05
2	B	141	ASP	C-N-CA	6.90	126.71	119.05
2	B	417	TRP	CA-C-O	-6.90	113.58	120.82
2	B	524	PHE	CA-CB-CG	6.89	120.69	113.80
1	C	367	SER	CA-C-O	6.88	129.51	121.46
2	D	371	GLU	CA-CB-CG	6.87	127.84	114.10
1	A	40	THR	O-C-N	-6.86	114.58	122.68
2	B	269	GLN	CB-CG-CD	6.86	124.26	112.60
2	B	87	TYR	CA-C-N	6.86	126.62	119.76
2	B	87	TYR	C-N-CA	6.86	126.62	119.76
2	D	511	PRO	N-CA-CB	6.85	109.07	103.32
2	B	413	ALA	CA-C-O	-6.85	113.63	120.82
2	D	398	PRO	O-C-N	-6.85	114.37	122.24
2	B	63	THR	O-C-N	-6.85	115.03	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	GLU	O-C-N	-6.84	114.21	122.22
1	C	166	THR	O-C-N	6.84	131.32	122.43
1	C	232	MET	O-C-N	-6.84	115.36	121.17
1	C	640	THR	CA-C-O	-6.83	113.64	120.82
1	A	405	GLY	O-C-N	-6.83	113.82	122.70
1	C	677	ARG	O-C-N	-6.83	115.22	121.37
1	C	98	SER	O-C-N	-6.83	115.04	122.07
1	C	646	GLU	O-C-N	-6.81	114.25	122.22
1	A	55	TYR	N-CA-C	6.81	120.85	112.54
2	D	34	GLN	CA-C-O	-6.81	113.85	121.00
2	D	146	ALA	CA-C-N	6.81	126.77	119.28
2	D	146	ALA	C-N-CA	6.81	126.77	119.28
2	B	424	GLU	CA-C-N	6.81	131.49	120.60
2	B	424	GLU	C-N-CA	6.81	131.49	120.60
1	C	644	ALA	CA-C-N	6.81	129.79	120.46
1	C	644	ALA	C-N-CA	6.81	129.79	120.46
1	C	61	LEU	CA-C-N	6.80	135.98	123.13
1	C	61	LEU	C-N-CA	6.80	135.98	123.13
2	D	229	PRO	CA-C-N	6.80	133.04	121.14
2	D	229	PRO	C-N-CA	6.80	133.04	121.14
1	C	55	TYR	N-CA-C	6.80	120.83	112.54
2	B	480	PRO	N-CA-CB	6.79	109.26	103.35
1	A	528	ASP	CA-C-N	6.78	134.67	122.06
1	A	528	ASP	C-N-CA	6.78	134.67	122.06
1	C	41	ALA	CA-C-N	6.78	133.00	121.14
1	C	41	ALA	C-N-CA	6.78	133.00	121.14
2	D	282	PHE	CA-CB-CG	6.76	120.56	113.80
2	B	59	LEU	O-C-N	-6.75	114.96	122.12
2	B	190	ALA	O-C-N	-6.75	114.35	122.11
2	D	362	PRO	N-CA-CB	6.74	109.22	103.35
1	A	79	TYR	CA-C-N	6.74	129.31	120.28
1	A	79	TYR	C-N-CA	6.74	129.31	120.28
2	D	141	ASP	CA-C-N	6.74	126.20	118.85
2	D	141	ASP	C-N-CA	6.74	126.20	118.85
1	A	212	TYR	CA-C-O	6.73	128.30	120.96
2	D	223	ARG	CA-C-O	6.73	127.69	120.55
1	C	692	ASP	CA-C-N	6.72	129.52	120.65
1	C	692	ASP	C-N-CA	6.72	129.52	120.65
2	B	63	THR	CA-C-O	6.71	128.34	120.69
1	C	177	LEU	CA-C-N	6.71	129.17	120.44
1	C	177	LEU	C-N-CA	6.71	129.17	120.44
1	C	214	PRO	N-CA-CB	6.70	110.46	103.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	485	ASN	N-CA-CB	6.70	120.00	109.82
1	A	230	ALA	O-C-N	-6.70	113.52	122.23
1	A	129	ASN	CA-C-O	6.69	126.07	119.51
1	C	449	ALA	O-C-N	-6.69	115.03	122.12
1	A	475	GLU	CA-C-O	6.68	123.64	119.29
2	B	251	GLU	CB-CG-CD	6.67	123.94	112.60
1	A	215	GLN	CB-CG-CD	6.67	123.94	112.60
1	A	412	LEU	CA-C-N	6.67	129.11	120.44
1	A	412	LEU	C-N-CA	6.67	129.11	120.44
1	C	359	HIS	CE1-NE2-CD2	-6.67	102.33	109.00
1	A	569	VAL	N-CA-C	-6.66	105.84	111.56
1	C	526	ASP	CA-C-N	6.66	126.60	119.28
1	C	526	ASP	C-N-CA	6.66	126.60	119.28
1	A	447	GLU	O-C-N	-6.65	114.44	122.22
2	B	54	THR	CA-C-O	-6.65	114.29	121.94
2	B	191	LYS	CA-C-N	6.65	133.36	121.66
2	B	191	LYS	C-N-CA	6.65	133.36	121.66
2	D	521	ARG	CA-C-N	6.65	129.49	120.38
2	D	521	ARG	C-N-CA	6.65	129.49	120.38
2	B	478	PRO	N-CA-CB	6.65	109.13	103.35
1	C	389	PHE	O-C-N	-6.64	115.18	122.09
2	D	637	ALA	CA-C-N	6.64	133.66	121.70
2	D	637	ALA	C-N-CA	6.64	133.66	121.70
1	A	333	GLY	CA-C-N	6.64	129.85	120.28
1	A	333	GLY	C-N-CA	6.64	129.85	120.28
2	B	307	ILE	CA-C-O	-6.64	114.19	121.29
2	D	90	VAL	CA-CB-CG2	6.63	121.68	110.40
1	A	277	VAL	O-C-N	-6.62	115.40	121.89
2	B	117	ASP	CA-CB-CG	6.62	119.22	112.60
2	B	176	ALA	CA-C-O	6.62	128.35	121.07
2	B	418	LYS	O-C-N	-6.62	115.10	122.12
1	A	677	ARG	CA-CB-CG	6.62	127.33	114.10
2	D	271	PHE	CA-C-O	-6.61	113.56	121.56
2	B	141	ASP	O-C-N	-6.61	115.02	121.56
1	C	132	VAL	CA-C-N	6.61	129.43	120.38
1	C	132	VAL	C-N-CA	6.61	129.43	120.38
1	C	539	GLY	CA-C-N	6.61	129.79	120.28
1	C	539	GLY	C-N-CA	6.61	129.79	120.28
1	C	696	LEU	CA-C-N	6.61	129.79	120.28
1	C	696	LEU	C-N-CA	6.61	129.79	120.28
1	C	262	ASP	O-C-N	-6.60	115.27	122.07
2	D	32	GLU	CA-C-N	6.59	129.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	32	GLU	C-N-CA	6.59	129.11	120.28
1	A	150	ARG	NH1-CZ-NH2	6.59	127.87	119.30
1	C	375	PRO	N-CA-CB	6.59	109.08	103.35
1	C	419	LYS	N-CA-CB	6.58	119.79	110.12
1	A	75	TYR	CA-C-N	6.58	129.39	120.38
1	A	75	TYR	C-N-CA	6.58	129.39	120.38
1	C	485	ASN	OD1-CG-ND2	6.58	129.18	122.60
1	A	276	ASN	O-C-N	-6.57	115.53	122.96
1	C	488	VAL	CB-CA-C	-6.57	103.59	111.81
2	B	525	GLY	CA-C-N	6.57	134.28	121.41
2	B	525	GLY	C-N-CA	6.57	134.28	121.41
2	B	251	GLU	CA-C-N	6.57	129.37	120.44
2	B	251	GLU	C-N-CA	6.57	129.37	120.44
1	C	633	LEU	O-C-N	-6.57	114.64	122.65
2	D	507	VAL	O-C-N	-6.57	113.87	122.47
1	A	231	ASN	O-C-N	-6.56	114.54	122.48
1	C	268	ARG	O-C-N	-6.56	114.55	122.22
1	A	352	ALA	O-C-N	-6.55	115.18	122.12
2	D	322	GLN	O-C-N	-6.55	115.50	123.30
1	C	573	GLU	CA-C-O	-6.55	113.86	121.07
1	C	449	ALA	CA-C-N	6.55	129.05	120.28
1	C	449	ALA	C-N-CA	6.55	129.05	120.28
2	D	425	LYS	CA-CB-CG	6.54	127.19	114.10
1	C	306	MET	CA-C-O	-6.54	113.49	120.42
1	C	327	THR	N-CA-C	6.54	120.17	109.06
1	A	285	SER	CA-C-O	6.54	128.79	121.40
2	B	269	GLN	CA-C-N	6.53	131.44	121.51
2	B	269	GLN	C-N-CA	6.53	131.44	121.51
2	B	456	ARG	O-C-N	-6.53	113.66	122.41
1	A	623	ASP	N-CA-C	6.53	120.11	111.75
1	C	5	PRO	N-CA-CB	6.53	109.12	103.31
1	A	591	GLU	CB-CG-CD	6.52	123.69	112.60
2	D	46	GLY	CA-C-N	6.52	129.41	120.67
2	D	46	GLY	C-N-CA	6.52	129.41	120.67
2	D	123	LYS	CA-C-N	6.52	129.34	120.54
2	D	123	LYS	C-N-CA	6.52	129.34	120.54
1	C	215	GLN	CA-C-N	6.51	125.95	118.85
1	C	215	GLN	C-N-CA	6.51	125.95	118.85
1	C	591	GLU	CA-C-N	6.51	129.00	120.28
1	C	591	GLU	C-N-CA	6.51	129.00	120.28
2	B	602	PHE	CA-CB-CG	6.50	120.31	113.80
2	D	21	LEU	CA-C-O	6.50	128.09	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	ARG	CA-C-O	6.50	127.50	120.94
1	A	343	ASN	CA-C-N	6.49	130.99	120.60
1	A	343	ASN	C-N-CA	6.49	130.99	120.60
2	B	558	LYS	N-CA-C	6.49	118.35	111.28
1	C	403	TRP	CA-C-N	6.49	131.58	121.26
1	C	403	TRP	C-N-CA	6.49	131.58	121.26
2	D	95	ARG	CA-C-O	-6.49	112.77	120.10
2	D	633	ILE	CA-C-O	-6.49	114.30	121.05
1	A	447	GLU	CA-C-N	6.49	128.87	120.44
1	A	447	GLU	C-N-CA	6.49	128.87	120.44
1	A	699	ASP	CA-CB-CG	6.49	119.09	112.60
2	B	513	VAL	N-CA-CB	6.48	120.63	111.82
2	D	272	THR	CA-C-N	6.48	131.69	120.68
2	D	272	THR	C-N-CA	6.48	131.69	120.68
2	D	605	ASP	CA-C-N	6.48	129.28	120.54
2	D	605	ASP	C-N-CA	6.48	129.28	120.54
2	D	43	LEU	O-C-N	-6.47	113.76	122.43
2	D	78	PRO	CA-C-N	6.47	129.83	120.38
2	D	78	PRO	C-N-CA	6.47	129.83	120.38
1	A	133	ALA	CA-C-N	6.47	132.30	120.79
1	A	133	ALA	C-N-CA	6.47	132.30	120.79
1	C	436	ALA	CA-C-O	6.47	127.28	120.42
1	A	558	ARG	CB-CG-CD	6.46	126.17	111.30
1	A	636	THR	CA-C-N	6.46	126.09	119.56
1	A	636	THR	C-N-CA	6.46	126.09	119.56
1	A	25	PHE	CA-C-O	6.46	127.35	120.70
1	C	587	VAL	CA-C-N	6.46	128.93	120.28
1	C	587	VAL	C-N-CA	6.46	128.93	120.28
2	B	86	GLY	CA-C-N	6.45	136.79	122.67
2	B	86	GLY	C-N-CA	6.45	136.79	122.67
2	B	231	SER	O-C-N	-6.45	115.02	122.89
2	B	337	TYR	CA-C-N	6.45	131.34	120.64
2	B	337	TYR	C-N-CA	6.45	131.34	120.64
1	C	54	VAL	O-C-N	-6.45	113.61	122.05
2	B	379	ALA	CA-C-O	-6.44	114.06	120.70
1	C	184	GLU	CA-C-N	6.44	134.04	122.06
1	C	184	GLU	C-N-CA	6.44	134.04	122.06
2	D	301	ARG	CA-C-O	-6.44	114.01	120.90
1	A	215	GLN	O-C-N	-6.43	113.92	121.32
1	A	41	ALA	CA-C-N	6.43	134.12	121.58
1	A	41	ALA	C-N-CA	6.43	134.12	121.58
1	C	23	ARG	NE-CZ-NH1	6.43	127.93	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	GLU	N-CA-C	6.43	120.38	112.54
2	B	146	ALA	CA-C-N	6.43	126.92	119.47
2	B	146	ALA	C-N-CA	6.43	126.92	119.47
2	D	278	ASP	CA-C-O	-6.42	110.70	119.05
1	C	93	SER	O-C-N	-6.42	114.05	122.59
1	A	597	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	C	672	LEU	CA-C-O	-6.41	114.08	120.82
1	A	590	PHE	O-C-N	-6.41	115.42	122.09
1	A	711	ILE	CA-C-N	6.41	126.17	119.05
1	A	711	ILE	C-N-CA	6.41	126.17	119.05
2	D	166	VAL	N-CA-CB	6.41	120.87	112.60
2	D	610	GLU	O-C-N	-6.41	115.32	122.12
1	A	5	PRO	N-CA-CB	6.41	108.89	103.25
2	D	308	GLY	N-CA-C	6.41	120.64	112.83
1	C	658	ALA	O-C-N	-6.40	114.66	122.34
1	A	53	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	434	MET	CA-C-N	6.40	131.85	121.74
2	B	434	MET	C-N-CA	6.40	131.85	121.74
2	D	590	ALA	CA-C-O	6.40	128.06	120.70
1	A	236	ASN	OD1-CG-ND2	6.40	129.00	122.60
2	B	243	ASN	CA-C-N	6.38	133.07	122.54
2	B	243	ASN	C-N-CA	6.38	133.07	122.54
1	C	678	PRO	CA-C-N	6.38	132.31	121.14
1	C	678	PRO	C-N-CA	6.38	132.31	121.14
2	D	304	TRP	CA-C-N	6.38	129.16	120.54
2	D	304	TRP	C-N-CA	6.38	129.16	120.54
1	C	40	THR	O-C-N	-6.38	114.87	122.65
2	D	251	GLU	CB-CG-CD	6.38	123.44	112.60
1	C	667	ALA	CA-C-N	6.37	128.73	120.44
1	C	667	ALA	C-N-CA	6.37	128.73	120.44
1	A	189	PRO	N-CA-CB	6.37	110.27	103.39
1	C	612	ARG	O-C-N	6.37	128.72	122.09
1	A	243	TYR	O-C-N	-6.36	115.47	122.09
1	A	274	GLY	N-CA-C	6.36	124.40	115.43
2	B	504	SER	N-CA-C	6.36	119.19	111.82
2	D	237	ASP	O-C-N	-6.36	113.64	122.41
2	D	397	ASP	CA-C-N	6.36	126.57	119.32
2	D	397	ASP	C-N-CA	6.36	126.57	119.32
1	A	285	SER	O-C-N	-6.35	115.48	123.17
2	D	268	GLU	O-C-N	-6.35	115.53	122.07
1	A	115	VAL	CB-CA-C	-6.34	103.28	110.96
2	B	586	LYS	CA-CB-CG	6.34	126.79	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	538	ALA	CA-C-N	6.34	132.65	120.66
2	D	538	ALA	C-N-CA	6.34	132.65	120.66
1	C	475	GLU	CA-C-O	6.34	124.68	119.36
1	C	245	MET	CA-C-O	-6.33	113.84	120.55
1	C	401	ASP	CA-C-N	6.33	126.24	119.28
1	C	401	ASP	C-N-CA	6.33	126.24	119.28
2	B	223	ARG	O-C-N	-6.32	114.83	122.22
2	B	401	GLY	O-C-N	-6.32	114.49	122.70
1	C	244	HIS	CA-C-N	6.32	128.74	120.28
1	C	244	HIS	C-N-CA	6.32	128.74	120.28
1	C	155	GLY	O-C-N	-6.31	115.06	122.45
2	B	342	ARG	NE-CZ-NH1	6.31	127.81	121.50
2	D	488	LEU	N-CA-C	6.31	119.37	109.96
1	A	122	HIS	CA-CB-CG	-6.31	107.49	113.80
1	C	51	ASN	CA-C-N	6.31	130.70	120.60
1	C	51	ASN	C-N-CA	6.31	130.70	120.60
2	D	237	ASP	CA-C-O	6.31	129.04	121.66
1	A	91	GLY	N-CA-C	-6.30	98.24	113.18
2	B	297	LEU	CA-C-N	6.30	129.24	120.29
2	B	297	LEU	C-N-CA	6.30	129.24	120.29
1	C	357	GLN	CA-C-N	6.30	135.96	121.34
1	C	357	GLN	C-N-CA	6.30	135.96	121.34
2	B	256	LEU	CA-C-N	6.30	128.62	120.44
2	B	256	LEU	C-N-CA	6.30	128.62	120.44
1	C	264	VAL	O-C-N	-6.30	115.76	121.87
1	C	305	ARG	N-CA-CB	6.30	119.14	110.01
2	B	488	LEU	N-CA-C	6.29	119.95	110.64
2	B	629	SER	O-C-N	-6.29	115.45	122.12
1	C	251	THR	O-C-N	-6.29	115.68	122.85
1	A	515	ILE	O-C-N	-6.29	115.75	121.91
2	D	457	LYS	CA-C-N	6.29	131.60	122.98
2	D	457	LYS	C-N-CA	6.29	131.60	122.98
1	A	170	ALA	O-C-N	-6.29	112.66	121.72
1	A	332	SER	O-C-N	-6.29	115.04	122.96
2	B	223	ARG	CA-C-N	6.29	132.85	122.73
2	B	223	ARG	C-N-CA	6.29	132.85	122.73
1	A	198	ASN	CA-CB-CG	6.28	118.88	112.60
1	C	70	PHE	CB-CA-C	-6.28	102.97	111.89
1	C	89	TYR	N-CA-CB	-6.28	100.58	110.06
1	A	269	ALA	O-C-N	-6.27	115.47	122.12
2	B	136	LEU	CA-C-O	6.27	127.36	120.71
1	A	61	LEU	CA-C-O	-6.27	110.90	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	TRP	O-C-N	-6.27	113.28	122.43
2	B	432	ALA	CA-C-N	6.27	129.32	120.42
2	B	432	ALA	C-N-CA	6.27	129.32	120.42
2	B	230	ASP	CA-C-N	6.26	129.76	120.87
2	B	230	ASP	C-N-CA	6.26	129.76	120.87
2	D	223	ARG	O-C-N	-6.26	115.48	122.12
2	B	190	ALA	CA-C-N	6.26	132.63	120.99
2	B	190	ALA	C-N-CA	6.26	132.63	120.99
2	B	274	THR	O-C-N	-6.25	115.49	122.12
1	A	64	TYR	CA-C-N	6.24	129.58	120.71
1	A	64	TYR	C-N-CA	6.24	129.58	120.71
1	A	418	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	C	435	LYS	N-CA-C	6.24	118.08	111.28
1	A	252	ALA	N-CA-C	6.24	118.08	111.28
2	D	510	ARG	CA-C-O	6.24	125.61	119.75
1	A	216	PRO	N-CA-CB	6.23	110.12	103.52
2	D	83	LYS	O-C-N	-6.23	115.05	122.15
1	C	281	ALA	CA-C-O	6.23	124.38	118.34
2	D	613	ILE	CA-C-O	6.23	127.23	120.57
1	A	675	LEU	CA-C-N	6.23	131.00	120.91
1	A	675	LEU	C-N-CA	6.23	131.00	120.91
1	C	504	ASP	CA-C-N	6.23	125.96	119.05
1	C	504	ASP	C-N-CA	6.23	125.96	119.05
1	C	577	THR	CA-C-N	6.23	125.72	119.24
1	C	577	THR	C-N-CA	6.23	125.72	119.24
2	B	610	GLU	CA-C-N	6.22	129.24	120.28
2	B	610	GLU	C-N-CA	6.22	129.24	120.28
2	B	439	THR	CA-C-N	6.22	128.52	120.44
2	B	439	THR	C-N-CA	6.22	128.52	120.44
2	D	228	SER	CA-C-N	6.22	126.76	120.04
2	D	228	SER	C-N-CA	6.22	126.76	120.04
2	B	173	GLY	O-C-N	-6.22	116.21	122.18
2	B	81	ALA	N-CA-C	-6.21	101.52	110.40
2	D	263	VAL	N-CA-CB	6.21	117.67	110.65
2	D	321	ARG	NH1-CZ-NH2	6.21	127.37	119.30
2	D	78	PRO	N-CA-CB	6.21	110.16	103.33
1	A	527	PRO	N-CA-CB	6.20	109.47	103.51
1	C	617	ILE	N-CA-CB	6.20	117.81	110.55
1	C	483	VAL	CA-C-O	-6.20	113.14	121.02
1	A	50	PHE	O-C-N	-6.20	115.17	123.23
1	C	141	VAL	CA-CB-CG1	6.20	120.94	110.40
1	A	537	ASP	CA-C-O	-6.20	113.98	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	ILE	O-C-N	-6.19	115.84	121.91
2	B	507	VAL	CA-C-N	6.19	129.08	120.29
2	B	507	VAL	C-N-CA	6.19	129.08	120.29
2	B	616	ARG	CD-NE-CZ	6.19	133.07	124.40
1	C	634	PHE	CA-CB-CG	6.19	119.99	113.80
1	C	668	LEU	CA-C-N	6.19	128.90	120.54
1	C	668	LEU	C-N-CA	6.19	128.90	120.54
1	A	63	THR	O-C-N	-6.19	114.02	122.81
1	A	149	MET	CA-C-N	6.19	128.49	120.44
1	A	149	MET	C-N-CA	6.19	128.49	120.44
1	A	685	GLY	O-C-N	6.18	128.98	123.60
1	A	689	PRO	CA-C-O	-6.18	114.37	121.36
1	A	203	GLU	CA-C-O	-6.18	113.87	120.42
2	B	31	THR	CA-C-O	6.18	128.69	121.46
2	B	268	GLU	CA-CB-CG	6.17	126.44	114.10
1	A	685	GLY	CA-C-O	-6.16	114.98	121.57
1	C	484	ASP	O-C-N	-6.16	115.72	123.05
1	A	438	GLU	CB-CG-CD	6.16	123.06	112.60
1	C	300	LYS	CA-C-O	6.16	127.49	120.90
2	D	272	THR	CA-C-O	6.16	129.43	121.67
2	D	200	ASP	CA-C-O	6.15	128.59	120.16
2	B	211	GLU	CA-C-O	6.15	124.70	119.66
1	A	7	PHE	N-CA-C	6.15	120.47	113.15
1	A	219	ARG	O-C-N	-6.14	115.15	122.15
1	C	282	PRO	O-C-N	-6.14	114.29	122.22
2	D	480	PRO	N-CA-CB	6.14	108.48	103.32
2	B	389	GLU	CA-C-O	6.14	126.73	119.67
2	D	353	GLY	O-C-N	-6.14	115.71	122.84
1	A	23	ARG	O-C-N	-6.14	114.72	122.27
2	B	162	THR	N-CA-C	6.14	118.90	108.90
1	A	262	ASP	CA-C-N	6.13	126.92	119.99
1	A	262	ASP	C-N-CA	6.13	126.92	119.99
1	C	98	SER	CA-C-O	6.13	127.26	120.82
1	A	300	LYS	O-C-N	-6.13	115.75	122.07
2	B	249	VAL	CA-C-O	-6.13	114.67	121.17
1	A	623	ASP	O-C-N	-6.13	115.22	122.20
2	B	44	ASN	CA-CB-CG	-6.13	106.47	112.60
1	C	369	ASP	O-C-N	-6.13	114.53	122.37
2	B	257	ALA	CA-C-N	6.12	128.40	120.44
2	B	257	ALA	C-N-CA	6.12	128.40	120.44
2	B	448	GLU	CA-C-O	-6.12	113.93	120.42
1	C	529	ARG	N-CA-CB	-6.12	101.07	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	GLN	CB-CA-C	-6.12	104.11	110.17
2	D	91	ALA	CA-C-O	6.11	125.95	120.02
1	A	430	VAL	CA-CB-CG1	6.11	120.79	110.40
2	B	624	VAL	CA-C-N	6.11	128.38	120.44
2	B	624	VAL	C-N-CA	6.11	128.38	120.44
2	D	543	PRO	N-CA-CB	6.11	108.67	103.35
1	C	434	ALA	CA-C-O	-6.10	114.42	120.82
1	C	412	LEU	O-C-N	-6.10	115.66	122.12
1	C	241	SER	N-CA-C	6.09	119.40	109.59
2	B	396	ASN	O-C-N	-6.09	115.44	122.93
1	C	637	PRO	O-C-N	-6.09	114.92	122.23
1	C	692	ASP	N-CA-C	6.09	120.57	113.20
2	D	328	TRP	O-C-N	-6.09	113.33	122.28
1	A	215	GLN	N-CA-CB	6.09	121.21	110.37
2	D	100	ARG	NE-CZ-NH2	-6.09	113.72	119.20
2	D	371	GLU	CB-CA-C	6.09	120.26	110.09
2	B	511	PRO	N-CA-CB	6.09	108.61	103.25
1	A	654	VAL	CA-C-N	-6.09	114.47	123.11
1	A	654	VAL	C-N-CA	-6.09	114.47	123.11
1	C	590	PHE	CA-C-N	6.09	128.35	120.44
1	C	590	PHE	C-N-CA	6.09	128.35	120.44
1	A	491	GLU	O-C-N	-6.08	114.78	122.27
2	B	422	GLU	CA-C-N	6.08	128.80	120.46
2	B	422	GLU	C-N-CA	6.08	128.80	120.46
2	D	355	ALA	N-CA-CB	6.08	118.92	109.97
1	C	311	LEU	O-C-N	-6.08	115.22	122.15
1	A	635	GLN	CA-C-N	-6.08	113.30	122.29
1	A	635	GLN	C-N-CA	-6.08	113.30	122.29
2	B	265	ALA	CA-C-O	-6.08	114.07	120.63
2	D	31	THR	CA-C-N	6.08	128.74	120.54
2	D	31	THR	C-N-CA	6.08	128.74	120.54
2	D	127	GLU	O-C-N	-6.08	114.51	122.59
2	B	39	VAL	CA-C-N	6.07	128.34	120.44
2	B	39	VAL	C-N-CA	6.07	128.34	120.44
1	C	568	GLY	N-CA-C	6.07	124.05	115.30
2	B	297	LEU	N-CA-CB	6.07	119.05	110.12
2	B	359	THR	CA-CB-OG1	-6.07	100.50	109.60
1	C	535	CYS	CA-C-O	6.06	126.98	120.55
1	A	262	ASP	O-C-N	-6.06	115.83	122.07
1	C	47	GLY	O-C-N	-6.06	117.60	122.81
1	A	575	LYS	O-C-N	-6.06	115.20	122.65
2	B	291	PHE	CA-CB-CG	-6.05	107.75	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	VAL	O-C-N	-6.05	115.59	121.83
1	C	430	VAL	CA-C-O	6.05	128.35	120.78
2	D	47	ARG	N-CA-C	6.05	118.39	109.50
1	A	669	ARG	CB-CG-CD	6.05	125.21	111.30
2	B	396	ASN	CA-CB-CG	-6.05	106.55	112.60
2	D	422	GLU	O-C-N	-6.05	115.31	122.20
1	C	206	VAL	O-C-N	-6.04	115.01	122.57
1	C	208	ASN	N-CA-C	6.04	119.95	112.58
2	D	588	ALA	N-CA-C	6.04	121.71	113.37
2	B	23	LEU	O-C-N	-6.04	115.87	121.79
1	A	352	ALA	CA-C-O	6.03	126.95	120.55
1	C	233	PRO	N-CA-CB	6.03	109.30	103.51
2	B	370	PRO	N-CA-CB	6.03	108.56	103.25
1	C	96	LYS	CA-C-O	-6.03	114.16	120.55
2	B	300	LEU	CA-C-O	-6.02	114.45	120.90
1	A	23	ARG	CA-C-N	6.02	128.84	120.29
1	A	23	ARG	C-N-CA	6.02	128.84	120.29
1	C	476	PRO	N-CA-CB	6.02	108.92	103.08
2	B	315	GLU	N-CA-C	6.01	119.44	111.75
2	B	375	PRO	N-CA-CB	6.01	109.94	103.33
1	C	246	GLN	OE1-CD-NE2	6.01	128.61	122.60
1	C	276	ASN	O-C-N	-6.00	116.01	122.85
2	B	264	ARG	O-C-N	-6.00	115.79	122.03
1	C	665	VAL	N-CA-C	6.00	119.55	112.35
1	A	638	GLU	CA-C-O	6.00	126.89	120.24
2	D	403	TYR	CA-C-O	6.00	127.11	120.82
2	B	374	PHE	CA-C-N	5.99	125.70	119.05
2	B	374	PHE	C-N-CA	5.99	125.70	119.05
1	C	640	THR	O-C-N	5.99	128.24	122.07
1	C	268	ARG	CA-C-N	5.99	128.23	120.44
1	C	268	ARG	C-N-CA	5.99	128.23	120.44
2	D	364	THR	CA-C-N	5.98	130.71	120.72
2	D	364	THR	C-N-CA	5.98	130.71	120.72
1	A	512	LEU	O-C-N	-5.97	115.92	122.07
2	D	67	VAL	CA-C-N	5.97	134.19	122.61
2	D	67	VAL	C-N-CA	5.97	134.19	122.61
2	D	327	SER	CA-C-O	5.97	127.73	120.92
1	A	24	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	A	151	GLU	CA-C-N	5.97	128.20	120.44
1	A	151	GLU	C-N-CA	5.97	128.20	120.44
2	D	628	SER	CA-C-N	5.96	128.27	120.28
2	D	628	SER	C-N-CA	5.96	128.27	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	PRO	O-C-N	-5.96	114.59	122.64
1	C	216	PRO	N-CA-CB	5.96	110.12	103.44
1	A	389	PHE	O-C-N	-5.96	115.80	122.12
1	A	521	ASN	O-C-N	-5.96	115.94	121.36
1	C	398	ARG	NH1-CZ-NH2	5.96	127.04	119.30
1	A	579	GLU	CA-C-N	5.95	128.06	120.56
1	A	579	GLU	C-N-CA	5.95	128.06	120.56
2	B	492	ARG	O-C-N	-5.95	115.83	122.86
2	D	348	PHE	O-C-N	-5.95	115.94	122.07
2	B	139	ARG	CA-C-O	-5.95	114.21	120.58
1	A	696	LEU	N-CA-C	5.95	118.25	111.11
1	A	720	LYS	CA-C-N	5.94	128.16	120.44
1	A	720	LYS	C-N-CA	5.94	128.16	120.44
1	C	497	VAL	O-C-N	-5.94	116.09	121.91
1	A	42	GLU	O-C-N	-5.93	113.77	122.43
1	C	198	ASN	N-CA-CB	-5.93	102.92	111.70
1	A	95	ALA	CA-C-O	-5.93	114.60	120.82
1	A	347	ARG	CD-NE-CZ	5.92	132.69	124.40
2	B	225	ALA	CA-C-N	5.92	128.54	120.54
2	B	225	ALA	C-N-CA	5.92	128.54	120.54
1	C	541	ALA	O-C-N	-5.92	113.62	122.39
1	A	122	HIS	CB-CA-C	-5.92	101.58	110.88
2	B	544	GLN	CA-C-N	-5.92	113.28	122.69
2	B	544	GLN	C-N-CA	-5.92	113.28	122.69
2	D	559	LYS	CA-C-N	5.92	128.13	120.44
2	D	559	LYS	C-N-CA	5.92	128.13	120.44
1	A	635	GLN	CA-CB-CG	5.91	125.93	114.10
2	B	45	ARG	CA-C-O	-5.91	112.05	120.51
1	C	146	ILE	CA-C-N	5.91	128.13	120.44
1	C	146	ILE	C-N-CA	5.91	128.13	120.44
2	B	36	GLU	CA-C-N	5.90	128.19	120.28
2	B	36	GLU	C-N-CA	5.90	128.19	120.28
1	C	131	ARG	NE-CZ-NH2	5.90	124.51	119.20
2	D	61	ARG	O-C-N	-5.89	115.33	122.22
1	C	526	ASP	CA-C-O	5.89	125.01	119.59
1	C	52	GLU	O-C-N	-5.89	114.73	122.39
1	C	241	SER	CA-C-N	5.89	132.95	121.41
1	C	241	SER	C-N-CA	5.89	132.95	121.41
1	A	677	ARG	O-C-N	-5.89	116.56	121.27
2	D	115	ASP	CA-C-N	5.88	125.09	118.97
2	D	115	ASP	C-N-CA	5.88	125.09	118.97
1	A	241	SER	N-CA-C	5.88	119.40	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	156	ILE	CA-C-N	5.87	127.18	119.84
1	C	156	ILE	C-N-CA	5.87	127.18	119.84
1	C	299	ALA	N-CA-CB	-5.87	101.47	110.16
2	B	180	VAL	CB-CA-C	-5.87	104.21	112.14
1	C	170	ALA	CA-C-N	5.87	128.50	120.46
1	C	170	ALA	C-N-CA	5.87	128.50	120.46
1	A	586	LEU	CA-C-N	5.87	128.07	120.56
1	A	586	LEU	C-N-CA	5.87	128.07	120.56
2	D	439	THR	CA-C-N	5.87	128.07	120.44
2	D	439	THR	C-N-CA	5.87	128.07	120.44
1	A	215	GLN	OE1-CD-NE2	-5.87	116.73	122.60
2	D	340	ILE	CA-C-N	5.87	128.62	120.29
2	D	340	ILE	C-N-CA	5.87	128.62	120.29
1	C	237	SER	CA-C-N	5.86	129.81	121.96
1	C	237	SER	C-N-CA	5.86	129.81	121.96
1	A	273	VAL	CA-C-N	5.86	132.16	121.85
1	A	273	VAL	C-N-CA	5.86	132.16	121.85
1	A	284	LEU	CA-C-O	-5.86	114.37	121.05
1	C	272	SER	CA-C-O	-5.86	112.40	119.49
2	D	293	THR	O-C-N	-5.86	115.81	122.08
2	B	461	THR	O-C-N	-5.86	116.03	123.06
2	D	387	ALA	CA-C-N	5.86	131.39	121.14
2	D	387	ALA	C-N-CA	5.86	131.39	121.14
2	B	125	ILE	N-CA-CB	5.85	116.77	110.62
1	A	393	GLU	N-CA-C	5.85	121.46	113.97
1	C	150	ARG	NH1-CZ-NH2	5.85	126.91	119.30
1	C	363	LEU	O-C-N	5.85	130.15	123.48
1	A	27	GLU	O-C-N	-5.85	115.08	122.27
2	B	397	ASP	O-C-N	-5.85	118.84	121.53
1	C	235	TRP	O-C-N	-5.85	116.41	123.13
2	D	409	THR	O-C-N	-5.84	116.01	122.09
1	C	304	ALA	O-C-N	-5.84	115.93	122.12
2	D	272	THR	N-CA-CB	5.84	118.86	110.45
1	C	359	HIS	CG-CD2-NE2	5.84	113.04	107.20
1	C	46	VAL	CA-C-N	-5.84	113.90	121.96
1	C	46	VAL	C-N-CA	-5.84	113.90	121.96
1	C	150	ARG	CB-CA-C	-5.84	101.10	110.79
2	B	409	THR	O-C-N	-5.84	116.06	122.07
1	A	595	GLY	N-CA-C	5.84	122.80	115.21
2	D	315	GLU	O-C-N	-5.83	114.61	122.43
1	A	612	ARG	CA-C-O	-5.83	114.66	120.90
1	C	261	ALA	O-C-N	-5.83	115.50	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	LEU	O-C-N	-5.83	116.07	122.07
2	B	315	GLU	O-C-N	-5.83	115.56	122.20
1	C	65	ALA	O-C-N	-5.83	115.98	122.86
1	A	66	GLY	N-CA-C	5.82	123.87	114.90
2	B	421	GLN	CA-C-O	-5.82	114.70	120.82
1	C	341	VAL	O-C-N	-5.82	114.42	122.05
1	A	688	ILE	CA-CB-CG1	5.82	120.29	110.40
1	C	430	VAL	CA-CB-CG1	5.82	120.29	110.40
2	B	20	THR	CA-C-O	-5.82	110.91	120.80
2	B	108	ASP	N-CA-CB	-5.82	100.94	110.42
1	C	527	PRO	CA-C-N	5.81	130.43	120.72
1	C	527	PRO	C-N-CA	5.81	130.43	120.72
1	A	236	ASN	CA-CB-CG	-5.81	106.79	112.60
1	A	507	LYS	CA-C-N	5.81	128.67	120.42
1	A	507	LYS	C-N-CA	5.81	128.67	120.42
1	C	587	VAL	O-C-N	-5.81	116.23	121.87
1	A	411	GLU	CA-C-O	-5.81	114.72	120.82
2	B	92	PRO	CA-C-N	5.81	133.55	123.91
2	B	92	PRO	C-N-CA	5.81	133.55	123.91
2	B	104	MET	CA-C-O	-5.81	114.27	120.42
1	C	453	THR	O-C-N	-5.80	116.09	122.07
2	B	587	ALA	CA-C-O	-5.80	114.69	120.90
1	A	683	THR	O-C-N	-5.80	115.62	123.10
2	D	574	TYR	CA-C-N	5.80	128.37	120.54
2	D	574	TYR	C-N-CA	5.80	128.37	120.54
1	C	28	LEU	N-CA-C	5.80	117.60	111.28
1	A	304	ALA	CA-C-N	5.79	127.97	120.44
1	A	304	ALA	C-N-CA	5.79	127.97	120.44
1	C	526	ASP	O-C-N	-5.79	114.51	121.12
2	B	223	ARG	NH1-CZ-NH2	5.79	126.83	119.30
1	C	85	THR	O-C-N	-5.79	116.26	123.04
1	C	20	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	319	ASN	CA-C-N	5.79	125.41	119.56
1	C	319	ASN	C-N-CA	5.79	125.41	119.56
1	C	617	ILE	CA-C-O	-5.79	115.03	121.17
1	A	374	LEU	CA-C-O	5.79	127.24	120.87
1	A	577	THR	CA-C-N	5.79	125.32	119.19
1	A	577	THR	C-N-CA	5.79	125.32	119.19
2	B	87	TYR	O-C-N	-5.78	115.87	121.94
2	B	510	ARG	CA-C-N	5.78	125.80	119.90
2	B	510	ARG	C-N-CA	5.78	125.80	119.90
2	B	189	PRO	N-CA-CB	5.78	109.32	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	723	ARG	CA-C-N	5.78	128.34	120.54
1	A	723	ARG	C-N-CA	5.78	128.34	120.54
1	A	369	ASP	O-C-N	-5.78	111.94	122.34
2	B	328	TRP	CA-C-O	5.78	126.65	120.24
2	D	379	ALA	CA-C-O	-5.77	114.76	120.82
1	C	268	ARG	CA-C-O	-5.77	113.58	120.10
1	C	534	LEU	N-CA-C	5.77	118.51	111.82
1	C	522	PRO	N-CA-CB	5.77	108.70	103.34
1	C	546	GLY	CA-C-O	-5.77	115.11	121.05
1	C	622	ALA	CA-C-N	5.77	129.83	120.60
1	C	622	ALA	C-N-CA	5.77	129.83	120.60
2	B	229	PRO	CA-C-N	5.76	130.35	120.72
2	B	229	PRO	C-N-CA	5.76	130.35	120.72
2	D	93	PHE	CA-CB-CG	-5.76	108.03	113.80
2	B	414	ASP	N-CA-C	5.75	117.55	111.28
1	A	466	GLY	CA-C-N	5.75	132.32	121.97
1	A	466	GLY	C-N-CA	5.75	132.32	121.97
2	B	560	SER	O-C-N	-5.75	115.59	122.15
2	D	331	LEU	CA-C-O	5.75	128.08	121.47
1	C	98	SER	CA-CB-OG	-5.75	99.60	111.10
1	C	677	ARG	CA-CB-CG	5.75	125.60	114.10
1	C	27	GLU	O-C-N	-5.75	116.03	122.12
1	C	342	TYR	O-C-N	-5.75	114.73	122.43
2	D	25	GLY	O-C-N	-5.75	116.60	122.17
1	C	707	PRO	N-CA-CB	5.74	108.30	103.25
2	D	123	LYS	O-C-N	-5.74	115.94	122.08
2	B	128	GLY	O-C-N	-5.74	116.67	122.18
1	C	559	TYR	CA-CB-CG	5.73	124.22	113.90
1	A	193	ALA	CA-C-O	5.73	126.79	120.71
1	C	205	MET	O-C-N	-5.73	115.84	122.03
1	C	172	LEU	O-C-N	-5.73	115.85	120.38
1	A	219	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	C	715	ALA	CA-C-N	5.73	127.78	120.56
1	C	715	ALA	C-N-CA	5.73	127.78	120.56
1	A	469	LYS	O-C-N	-5.72	116.89	123.42
1	C	562	GLN	O-C-N	-5.72	116.80	123.27
1	C	284	LEU	CA-C-O	-5.72	114.34	120.92
1	C	642	ARG	O-C-N	-5.72	116.14	122.09
1	A	612	ARG	CA-C-N	5.72	126.33	119.98
1	A	612	ARG	C-N-CA	5.72	126.33	119.98
2	B	437	HIS	CA-C-N	5.72	128.54	120.42
2	B	437	HIS	C-N-CA	5.72	128.54	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	SER	O-C-N	-5.72	116.18	122.07
2	D	434	MET	N-CA-C	5.72	118.25	111.33
1	C	529	ARG	CB-CG-CD	-5.71	98.17	111.30
2	B	78	PRO	N-CA-CB	5.71	109.77	103.26
2	D	44	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	158	LEU	N-CA-C	5.70	120.08	113.18
1	C	32	ALA	N-CA-C	5.70	119.34	112.38
1	C	402	PRO	CB-CA-C	-5.70	103.31	112.21
1	C	671	GLU	CB-CG-CD	5.70	122.30	112.60
1	C	328	HIS	N-CA-C	-5.70	102.08	110.52
1	A	358	GLY	CA-C-N	5.70	130.84	122.63
1	A	358	GLY	C-N-CA	5.70	130.84	122.63
1	A	200	ILE	O-C-N	-5.69	114.27	122.12
2	B	607	ALA	O-C-N	-5.69	116.21	122.07
2	D	397	ASP	CA-C-O	5.69	127.95	120.16
1	C	664	LEU	N-CA-C	5.69	117.16	111.07
2	B	222	ARG	NE-CZ-NH1	5.68	127.19	121.50
1	C	350	ILE	N-CA-C	5.68	116.46	110.72
2	D	54	THR	N-CA-C	-5.68	102.35	110.59
2	D	127	GLU	CA-C-N	5.68	126.39	120.03
2	D	127	GLU	C-N-CA	5.68	126.39	120.03
1	A	589	GLU	O-C-N	-5.68	116.22	122.07
2	B	228	SER	CA-C-N	5.68	125.78	119.87
2	B	228	SER	C-N-CA	5.68	125.78	119.87
2	B	520	THR	O-C-N	-5.68	116.25	122.84
2	B	637	ALA	CA-C-N	5.68	131.92	121.70
2	B	637	ALA	C-N-CA	5.68	131.92	121.70
1	C	394	SER	O-C-N	-5.68	115.28	122.27
2	D	571	ALA	CA-C-N	5.68	128.21	120.54
2	D	571	ALA	C-N-CA	5.68	128.21	120.54
1	A	104	ARG	CG-CD-NE	5.68	124.49	112.00
2	D	601	GLU	O-C-N	-5.68	114.62	122.46
2	D	383	GLY	CA-C-N	5.67	128.23	120.46
2	D	383	GLY	C-N-CA	5.67	128.23	120.46
2	B	607	ALA	CA-C-N	5.67	127.81	120.44
2	B	607	ALA	C-N-CA	5.67	127.81	120.44
1	C	78	MET	CA-C-O	5.67	128.62	120.51
1	C	680	ILE	O-C-N	5.67	129.18	122.66
1	C	511	ALA	O-C-N	-5.67	116.11	122.12
1	A	721	LYS	CA-C-N	5.67	127.81	120.44
1	A	721	LYS	C-N-CA	5.67	127.81	120.44
2	B	528	GLU	CA-C-N	5.67	126.27	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	528	GLU	C-N-CA	5.67	126.27	119.98
1	C	218	MET	O-C-N	-5.67	115.69	122.15
1	A	266	TYR	N-CA-C	5.66	118.22	111.71
1	C	408	TYR	CA-C-N	5.66	128.46	120.42
1	C	408	TYR	C-N-CA	5.66	128.46	120.42
2	B	328	TRP	CA-C-N	5.66	128.43	120.28
2	B	328	TRP	C-N-CA	5.66	128.43	120.28
1	A	49	LEU	O-C-N	-5.66	116.97	123.42
1	C	173	PRO	N-CA-CB	5.66	109.29	103.23
1	C	222	SER	CA-CB-OG	-5.66	99.78	111.10
1	A	398	ARG	N-CA-C	5.66	119.44	112.54
1	C	592	GLN	CB-CA-C	-5.66	101.40	110.79
2	D	142	PRO	N-CA-CB	5.66	109.78	103.44
1	C	215	GLN	CB-CG-CD	5.66	122.22	112.60
1	A	107	ALA	CA-C-N	5.66	132.29	122.56
1	A	107	ALA	C-N-CA	5.66	132.29	122.56
1	A	29	ALA	CA-C-N	5.65	127.79	120.44
1	A	29	ALA	C-N-CA	5.65	127.79	120.44
1	C	466	GLY	O-C-N	-5.65	115.25	122.43
1	A	206	VAL	CA-CB-CG1	5.65	120.01	110.40
2	D	248	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	99	ASN	CB-CG-ND2	5.65	124.87	116.40
2	B	602	PHE	CA-C-N	5.64	132.47	121.41
2	B	602	PHE	C-N-CA	5.64	132.47	121.41
2	D	28	PRO	N-CA-CB	5.64	108.27	103.19
1	A	467	VAL	CA-C-O	-5.64	113.73	120.78
2	D	92	PRO	N-CA-CB	5.63	108.80	102.60
1	C	91	GLY	N-CA-C	-5.63	99.83	113.18
1	C	703	GLU	CA-CB-CG	5.63	125.37	114.10
2	D	89	GLY	O-C-N	-5.63	115.34	122.32
1	A	221	ILE	CB-CA-C	-5.62	104.77	111.97
2	B	617	LEU	N-CA-CB	5.62	119.38	110.55
2	D	628	SER	O-C-N	-5.62	116.16	122.12
1	A	172	LEU	CA-C-N	5.62	125.29	119.05
1	A	172	LEU	C-N-CA	5.62	125.29	119.05
1	A	684	VAL	CB-CA-C	-5.62	102.13	110.33
2	B	246	ALA	CA-C-O	-5.62	115.69	121.87
2	B	237	ASP	O-C-N	-5.61	115.05	122.57
2	D	394	ARG	O-C-N	-5.61	114.71	122.46
1	C	73	GLY	CA-C-N	5.61	125.14	119.19
1	C	73	GLY	C-N-CA	5.61	125.14	119.19
2	D	83	LYS	CA-C-O	5.61	126.36	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	82	PRO	N-CA-CB	5.61	108.23	103.35
1	A	246	GLN	CB-CG-CD	5.60	122.12	112.60
1	C	121	THR	O-C-N	-5.60	116.26	122.09
2	D	147	PRO	N-CA-CB	5.60	109.44	103.39
2	D	419	GLU	CB-CG-CD	5.60	122.12	112.60
2	D	342	ARG	CA-C-O	-5.60	114.61	120.55
2	D	333	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	A	400	ILE	O-C-N	-5.59	116.56	122.83
1	C	350	ILE	O-C-N	-5.59	116.07	121.83
1	C	727	ASP	O-C-N	-5.59	115.50	122.83
1	A	252	ALA	CA-C-N	5.59	128.81	120.31
1	A	252	ALA	C-N-CA	5.59	128.81	120.31
2	B	71	ASP	CA-CB-CG	-5.59	107.01	112.60
2	B	477	LYS	CA-CB-CG	5.58	125.27	114.10
2	B	633	ILE	O-C-N	-5.58	116.42	121.89
1	A	142	ALA	O-C-N	-5.58	115.23	122.77
1	A	552	LEU	CA-C-N	5.58	128.32	120.28
1	A	552	LEU	C-N-CA	5.58	128.32	120.28
2	B	131	ARG	CA-C-O	5.58	127.92	121.34
1	A	485	ASN	CB-CG-ND2	-5.58	108.03	116.40
1	C	524	ASP	CA-CB-CG	5.58	118.18	112.60
2	D	622	ASP	CA-CB-CG	5.58	118.18	112.60
2	B	258	THR	CA-C-N	5.58	126.13	119.94
2	B	258	THR	C-N-CA	5.58	126.13	119.94
2	B	124	ALA	CA-C-O	5.58	126.67	120.82
2	D	444	ALA	CA-C-N	5.58	127.69	120.44
2	D	444	ALA	C-N-CA	5.58	127.69	120.44
1	A	413	THR	CA-C-N	5.57	127.75	120.28
1	A	413	THR	C-N-CA	5.57	127.75	120.28
1	A	670	LYS	CA-CB-CG	-5.57	102.95	114.10
1	C	28	LEU	CA-C-N	5.57	128.20	120.29
1	C	28	LEU	C-N-CA	5.57	128.20	120.29
1	A	423	HIS	CA-CB-CG	5.57	119.37	113.80
1	A	574	VAL	N-CA-CB	5.57	118.68	111.83
1	C	99	ASN	CA-CB-CG	5.57	118.17	112.60
1	C	283	ARG	N-CA-C	5.57	119.70	113.02
1	C	589	GLU	CA-C-O	5.57	126.45	120.55
2	D	180	VAL	CB-CA-C	-5.57	104.53	112.22
1	A	319	ASN	CA-C-O	5.57	125.84	119.61
1	A	379	SER	CA-C-O	5.57	126.32	120.42
2	D	41	LYS	CA-C-O	-5.56	114.65	120.55
2	B	86	GLY	CA-C-O	5.56	128.37	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	LEU	CA-C-O	5.56	126.31	120.42
2	B	122	ARG	CA-C-N	5.56	127.66	120.44
2	B	122	ARG	C-N-CA	5.56	127.66	120.44
2	B	343	GLY	O-C-N	-5.56	116.85	122.19
1	C	65	ALA	N-CA-C	-5.56	102.67	110.50
1	C	91	GLY	O-C-N	-5.55	115.48	122.70
1	C	153	PHE	CA-CB-CG	-5.55	108.25	113.80
2	D	84	LYS	CA-CB-CG	5.55	125.21	114.10
2	B	351	SER	O-C-N	-5.55	116.09	122.09
2	B	588	ALA	N-CA-C	5.55	119.75	113.15
1	C	351	GLU	O-C-N	-5.55	116.24	122.12
1	A	521	ASN	CA-C-O	5.55	128.24	120.64
2	D	50	GLU	CA-C-N	5.55	130.77	122.23
2	D	50	GLU	C-N-CA	5.55	130.77	122.23
2	D	78	PRO	O-C-N	-5.55	115.58	122.23
2	D	285	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	131	ARG	CD-NE-CZ	5.54	132.16	124.40
1	A	222	SER	O-C-N	-5.54	115.73	122.22
1	A	703	GLU	CA-CB-CG	5.54	125.19	114.10
1	C	186	GLY	CA-C-O	5.54	125.95	119.19
1	C	577	THR	CA-CB-CG2	5.54	119.92	110.50
1	A	4	LEU	CA-C-O	5.54	127.75	120.16
2	D	446	ASN	CA-CB-CG	-5.54	107.06	112.60
2	D	448	GLU	CA-C-N	5.54	128.26	120.28
2	D	448	GLU	C-N-CA	5.54	128.26	120.28
2	D	328	TRP	N-CA-CB	5.54	118.51	110.26
1	A	714	SER	CA-C-N	5.53	128.00	120.54
1	A	714	SER	C-N-CA	5.53	128.00	120.54
2	D	559	LYS	O-C-N	-5.53	116.26	122.12
1	A	687	VAL	O-C-N	-5.53	116.15	122.62
1	A	150	ARG	CD-NE-CZ	5.53	132.14	124.40
2	D	634	LEU	N-CA-C	5.53	119.77	113.19
2	B	544	GLN	CA-CB-CG	5.51	125.13	114.10
1	A	261	ALA	N-CA-C	-5.51	105.35	111.36
2	D	134	THR	N-CA-CB	5.51	118.33	110.67
2	D	457	LYS	CA-C-O	5.51	125.74	119.18
1	A	616	VAL	CA-CB-CG1	5.51	119.77	110.40
1	C	7	PHE	N-CA-C	5.51	119.71	113.15
1	C	721	LYS	O-C-N	-5.51	115.87	122.15
1	C	674	LYS	O-C-N	-5.50	115.06	122.43
2	D	190	ALA	CA-C-N	5.50	129.41	120.60
2	D	190	ALA	C-N-CA	5.50	129.41	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	512	LYS	CA-CB-CG	5.50	125.10	114.10
1	A	150	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	B	498	GLU	CA-C-N	5.50	127.64	120.28
2	B	498	GLU	C-N-CA	5.50	127.64	120.28
1	C	359	HIS	ND1-CE1-NE2	5.50	113.90	108.40
1	A	427	VAL	O-C-N	-5.49	116.45	121.94
2	B	159	LEU	N-CA-C	5.49	119.08	112.38
2	B	280	ILE	N-CA-C	5.49	116.64	108.23
1	C	137	GLY	O-C-N	-5.49	115.05	122.35
2	B	521	ARG	O-C-N	-5.49	115.80	122.22
1	C	497	VAL	CA-C-N	5.48	127.94	120.54
1	C	497	VAL	C-N-CA	5.48	127.94	120.54
1	A	319	ASN	CA-C-N	5.48	125.00	119.19
1	A	319	ASN	C-N-CA	5.48	125.00	119.19
1	C	137	GLY	CA-C-N	5.48	133.31	121.64
1	C	137	GLY	C-N-CA	5.48	133.31	121.64
1	C	15	ALA	CA-C-O	5.48	127.67	120.16
2	D	341	LEU	O-C-N	-5.48	115.90	122.15
1	C	140	GLY	CA-C-N	5.48	128.52	120.91
1	C	140	GLY	C-N-CA	5.48	128.52	120.91
1	A	334	TRP	O-C-N	-5.47	115.81	122.22
1	A	633	LEU	CA-C-N	5.47	130.34	122.40
1	A	633	LEU	C-N-CA	5.47	130.34	122.40
1	C	597	ARG	NE-CZ-NH2	-5.47	114.27	119.20
1	A	320	PRO	O-C-N	-5.47	114.88	122.27
1	A	521	ASN	N-CA-C	5.47	119.16	108.21
1	C	199	ASP	OD1-CG-OD2	-5.47	109.76	122.90
1	A	422	GLY	CA-C-N	5.47	127.61	120.28
1	A	422	GLY	C-N-CA	5.47	127.61	120.28
2	D	633	ILE	O-C-N	-5.47	116.53	121.89
1	C	676	GLY	O-C-N	-5.47	115.93	122.33
1	A	379	SER	O-C-N	-5.47	115.92	122.15
2	D	279	THR	CA-C-N	5.46	129.82	122.93
2	D	279	THR	C-N-CA	5.46	129.82	122.93
2	D	558	LYS	O-C-N	-5.46	116.41	122.09
1	C	471	ARG	CA-CB-CG	5.46	125.03	114.10
2	D	425	LYS	O-C-N	-5.46	114.31	122.39
1	A	641	ALA	O-C-N	-5.46	116.24	122.08
2	D	507	VAL	CA-C-O	5.46	128.52	121.80
1	C	213	PRO	N-CA-CB	5.46	108.37	103.08
2	D	202	ILE	CA-C-N	5.46	126.00	119.94
2	D	202	ILE	C-N-CA	5.46	126.00	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	483	PRO	N-CA-CB	5.46	108.16	103.36
2	D	363	PHE	CA-C-N	5.46	134.28	121.52
2	D	363	PHE	C-N-CA	5.46	134.28	121.52
1	A	666	PRO	N-CA-CB	5.45	109.55	103.44
2	B	533	PRO	CA-C-N	5.45	127.64	120.60
2	B	533	PRO	C-N-CA	5.45	127.64	120.60
1	C	582	GLU	CA-C-O	-5.45	114.77	120.55
2	D	26	ASP	N-CA-C	5.45	119.68	113.19
1	C	576	ASN	N-CA-C	5.45	118.91	111.39
1	C	688	ILE	CA-CB-CG1	5.45	119.66	110.40
2	D	292	LEU	O-C-N	-5.45	116.20	122.09
1	A	526	ASP	CA-C-N	5.44	125.06	119.56
1	A	526	ASP	C-N-CA	5.44	125.06	119.56
2	B	110	ARG	CD-NE-CZ	5.44	132.02	124.40
2	B	360	THR	CA-C-N	-5.44	112.41	120.68
2	B	360	THR	C-N-CA	-5.44	112.41	120.68
1	C	594	GLU	CB-CG-CD	5.44	121.85	112.60
2	D	397	ASP	O-C-N	-5.44	115.07	121.32
1	C	447	GLU	O-C-N	-5.44	115.86	122.22
1	A	447	GLU	CA-C-O	5.43	126.24	120.10
2	B	606	ALA	N-CA-C	5.43	116.88	111.07
1	C	8	ASP	CA-C-N	5.43	131.91	121.54
1	C	8	ASP	C-N-CA	5.43	131.91	121.54
1	C	50	PHE	O-C-N	-5.43	116.84	123.30
2	D	229	PRO	CA-C-O	5.43	125.74	118.90
1	A	134	GLY	CA-C-O	-5.43	113.10	119.50
1	A	444	MET	CB-CA-C	-5.43	101.63	110.85
1	A	716	ILE	CA-C-O	-5.43	115.42	121.17
1	C	219	ARG	O-C-N	-5.43	116.37	122.12
1	C	599	ARG	O-C-N	5.42	129.69	123.29
1	A	512	LEU	CA-C-O	5.42	126.51	120.82
1	C	579	GLU	CA-C-N	5.42	127.39	120.56
1	C	579	GLU	C-N-CA	5.42	127.39	120.56
1	A	301	LEU	CA-C-O	-5.42	114.81	120.55
1	C	465	ILE	N-CA-C	5.42	116.68	109.37
1	C	494	ALA	N-CA-C	5.42	117.19	111.28
2	D	337	TYR	O-C-N	-5.42	115.88	122.22
1	A	420	ALA	CA-C-O	-5.42	113.74	119.97
1	C	333	GLY	CA-C-O	5.42	126.33	120.75
1	C	360	THR	CA-CB-OG1	-5.42	101.48	109.60
1	A	644	ALA	CA-C-N	5.41	127.49	120.56
1	A	644	ALA	C-N-CA	5.41	127.49	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	469	LYS	O-C-N	-5.41	116.78	123.33
1	C	158	LEU	CA-C-N	5.41	129.88	120.68
1	C	158	LEU	C-N-CA	5.41	129.88	120.68
1	C	194	GLY	O-C-N	-5.41	118.09	124.15
1	A	665	VAL	N-CA-C	5.41	120.55	108.88
1	C	290	ILE	CA-CB-CG1	5.41	119.59	110.40
2	D	346	ALA	CA-C-O	-5.41	115.13	120.70
1	C	262	ASP	CA-C-N	5.40	125.98	119.98
1	C	262	ASP	C-N-CA	5.40	125.98	119.98
2	D	222	ARG	O-C-N	-5.40	115.62	122.27
2	B	23	LEU	CA-C-O	5.40	125.34	119.40
1	C	398	ARG	N-CA-C	5.40	117.17	111.28
2	D	36	GLU	O-C-N	-5.40	116.47	122.09
1	C	597	ARG	NE-CZ-NH1	5.40	126.90	121.50
2	D	357	SER	O-C-N	-5.40	116.60	123.24
1	A	390	LEU	O-C-N	-5.40	116.00	122.15
1	C	135	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	27	GLU	CA-C-O	5.39	126.17	119.97
1	A	66	GLY	CA-C-O	5.39	126.59	119.58
2	B	335	ASP	CA-C-N	5.39	124.91	119.19
2	B	335	ASP	C-N-CA	5.39	124.91	119.19
2	B	633	ILE	CA-C-O	-5.39	115.44	121.05
2	B	66	THR	O-C-N	-5.39	116.08	122.65
1	A	440	GLY	CA-C-N	5.39	124.64	120.33
1	A	440	GLY	C-N-CA	5.39	124.64	120.33
1	A	310	LYS	CA-C-O	-5.38	115.17	120.82
2	B	116	PRO	N-CA-CB	5.38	109.25	103.33
2	B	191	LYS	O-C-N	-5.38	115.27	122.43
1	C	102	TYR	N-CA-CB	5.38	118.14	110.06
1	C	130	PRO	N-CA-CB	5.38	109.20	103.39
1	C	185	GLN	CA-C-N	5.38	129.69	121.51
1	C	185	GLN	C-N-CA	5.38	129.69	121.51
1	C	320	PRO	CA-C-N	5.38	129.71	120.72
1	C	320	PRO	C-N-CA	5.38	129.71	120.72
1	C	341	VAL	N-CA-C	5.38	119.57	112.04
1	C	404	SER	O-C-N	5.38	130.44	123.07
2	D	56	ALA	CA-C-N	5.38	127.49	120.28
2	D	56	ALA	C-N-CA	5.38	127.49	120.28
2	B	327	SER	N-CA-C	5.38	117.50	109.59
1	A	14	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	486	SER	CA-C-N	5.38	129.82	120.68
1	A	486	SER	C-N-CA	5.38	129.82	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	327	SER	N-CA-C	5.38	118.11	110.10
1	A	349	CYS	O-C-N	-5.38	116.53	122.07
2	B	138	LEU	N-CA-CB	-5.38	102.13	110.57
2	D	538	ALA	O-C-N	-5.38	113.77	122.42
2	B	107	TRP	N-CA-C	-5.37	102.21	109.95
2	D	200	ASP	CA-C-N	5.37	124.56	118.97
2	D	200	ASP	C-N-CA	5.37	124.56	118.97
2	D	299	ALA	N-CA-CB	5.37	118.01	110.12
1	C	69	PRO	CA-C-N	5.37	129.98	122.36
1	C	69	PRO	C-N-CA	5.37	129.98	122.36
1	C	484	ASP	CA-C-O	-5.37	114.96	120.54
2	D	269	GLN	N-CA-C	5.37	120.78	113.37
2	D	348	PHE	CA-C-N	5.37	128.01	120.28
2	D	348	PHE	C-N-CA	5.37	128.01	120.28
1	A	183	GLU	CA-C-N	5.37	129.68	120.72
1	A	183	GLU	C-N-CA	5.37	129.68	120.72
1	A	615	LYS	O-C-N	-5.37	116.43	122.12
1	A	674	LYS	CA-CB-CG	5.37	124.83	114.10
2	B	238	ALA	CA-C-N	5.37	129.68	120.72
2	B	238	ALA	C-N-CA	5.37	129.68	120.72
2	B	441	VAL	CA-C-O	-5.37	115.09	121.05
2	D	248	ASP	CA-C-O	-5.37	115.17	120.70
2	D	21	LEU	O-C-N	-5.36	116.77	123.04
1	C	189	PRO	O-C-N	-5.36	115.30	122.22
2	D	610	GLU	CA-C-N	5.36	128.00	120.28
2	D	610	GLU	C-N-CA	5.36	128.00	120.28
1	C	415	ASP	CA-C-O	-5.36	114.87	120.55
1	C	585	GLU	O-C-N	-5.36	116.55	122.07
2	D	250	ALA	N-CA-CB	5.36	117.93	109.94
2	D	492	ARG	O-C-N	-5.36	116.22	122.81
2	B	50	GLU	CB-CG-CD	5.36	121.71	112.60
2	B	479	PHE	CA-CB-CG	5.36	119.16	113.80
2	D	495	GLU	O-C-N	-5.36	115.68	122.27
1	A	101	PHE	O-C-N	-5.36	116.52	122.09
1	A	197	GLN	O-C-N	-5.36	116.46	122.03
1	A	385	ASN	CA-CB-CG	5.36	117.96	112.60
2	B	308	GLY	O-C-N	-5.36	115.74	122.70
2	B	142	PRO	N-CA-CB	5.36	109.22	103.33
1	C	528	ASP	O-C-N	-5.36	115.25	122.43
2	D	298	ARG	NH1-CZ-NH2	-5.36	112.34	119.30
1	A	645	VAL	O-C-N	-5.35	116.33	121.90
1	C	70	PHE	O-C-N	-5.35	115.91	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	VAL	CA-C-O	-5.35	114.84	120.57
1	A	670	LYS	CA-C-O	-5.35	113.82	119.97
2	B	233	ALA	CA-C-N	5.35	129.67	122.93
2	B	233	ALA	C-N-CA	5.35	129.67	122.93
2	B	514	PHE	O-C-N	-5.34	116.45	123.02
2	B	613	ILE	CA-C-N	5.34	132.00	121.58
2	B	613	ILE	C-N-CA	5.34	132.00	121.58
1	A	430	VAL	N-CA-CB	-5.34	105.17	112.28
2	D	189	PRO	N-CA-CB	5.34	108.86	103.25
1	A	97	GLU	CA-C-N	5.34	127.38	120.44
1	A	97	GLU	C-N-CA	5.34	127.38	120.44
1	C	629	ASP	CA-CB-CG	-5.34	107.26	112.60
2	D	424	GLU	CA-C-N	5.34	132.62	121.94
2	D	424	GLU	C-N-CA	5.34	132.62	121.94
2	B	423	VAL	CA-C-N	5.34	129.71	120.58
2	B	423	VAL	C-N-CA	5.34	129.71	120.58
2	B	498	GLU	O-C-N	-5.34	116.06	122.15
1	A	233	PRO	N-CA-CB	5.33	108.63	103.51
1	C	122	HIS	CB-CA-C	-5.33	102.51	110.88
2	D	413	ALA	O-C-N	-5.33	116.58	122.07
2	B	249	VAL	CA-C-N	5.33	127.86	120.29
2	B	249	VAL	C-N-CA	5.33	127.86	120.29
1	C	178	TYR	CA-C-N	5.33	127.76	120.46
1	C	178	TYR	C-N-CA	5.33	127.76	120.46
1	C	207	ARG	CB-CG-CD	5.33	123.55	111.30
1	C	389	PHE	CA-C-O	5.33	126.60	120.90
1	C	518	ALA	CB-CA-C	-5.33	102.52	110.88
2	B	314	ASP	CA-CB-CG	5.32	117.92	112.60
2	D	405	VAL	CA-C-O	-5.32	115.21	120.85
2	D	505	THR	CA-C-N	5.32	128.40	120.31
2	D	505	THR	C-N-CA	5.32	128.40	120.31
1	C	253	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	588	GLU	O-C-N	-5.32	116.48	122.12
2	B	55	PHE	O-C-N	-5.31	116.60	122.07
1	C	162	SER	O-C-N	-5.31	117.00	123.27
1	A	484	ASP	O-C-N	-5.31	116.73	123.05
2	B	449	ARG	CA-C-N	5.31	127.40	120.28
2	B	449	ARG	C-N-CA	5.31	127.40	120.28
1	A	380	ALA	O-C-N	-5.31	116.49	122.12
1	C	117	PHE	O-C-N	-5.31	117.00	123.10
1	C	633	LEU	CA-C-O	5.31	128.04	121.99
1	A	631	GLY	CA-C-N	5.30	125.76	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	GLY	C-N-CA	5.30	125.76	120.14
1	C	350	ILE	CA-C-O	5.30	126.47	120.85
1	C	150	ARG	NE-CZ-NH1	-5.30	116.20	121.50
2	B	425	LYS	CA-C-N	5.30	132.54	121.94
2	B	425	LYS	C-N-CA	5.30	132.54	121.94
2	B	493	ASP	CA-C-O	-5.30	114.93	120.55
1	C	150	ARG	CA-C-N	5.30	127.81	120.29
1	C	150	ARG	C-N-CA	5.30	127.81	120.29
1	A	105	ASN	CA-C-O	-5.30	115.26	120.82
1	A	642	ARG	N-CA-C	5.30	117.05	111.28
2	B	154	LEU	O-C-N	-5.30	115.56	122.39
2	B	377	ARG	O-C-N	-5.30	116.50	122.12
2	B	628	SER	CA-C-O	-5.29	114.81	120.42
2	D	477	LYS	CA-C-N	5.29	125.30	119.90
2	D	477	LYS	C-N-CA	5.29	125.30	119.90
2	B	397	ASP	CA-C-O	5.29	124.49	120.26
1	A	97	GLU	CB-CG-CD	-5.29	103.61	112.60
1	A	397	THR	O-C-N	-5.29	114.90	122.41
2	B	264	ARG	CD-NE-CZ	5.29	131.80	124.40
1	C	369	ASP	CA-C-N	5.28	127.62	120.38
1	C	369	ASP	C-N-CA	5.28	127.62	120.38
2	D	288	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	289	GLY	O-C-N	-5.28	116.87	123.21
2	B	124	ALA	CA-C-N	5.28	127.69	120.77
2	B	124	ALA	C-N-CA	5.28	127.69	120.77
2	D	97	THR	N-CA-C	-5.28	105.66	112.68
1	C	320	PRO	N-CA-CB	5.28	108.58	103.51
1	C	662	LEU	CA-C-O	-5.28	113.90	119.97
1	C	372	ILE	N-CA-CB	-5.27	103.01	111.82
1	A	156	ILE	CA-C-N	5.27	126.43	119.84
1	A	156	ILE	C-N-CA	5.27	126.43	119.84
2	D	48	PRO	N-CA-CB	5.27	108.19	103.08
2	D	88	PRO	CB-CA-C	-5.27	103.42	110.85
2	D	208	GLN	CA-C-O	5.27	125.36	119.41
1	A	320	PRO	CB-CA-C	-5.27	104.42	112.11
1	A	531	LEU	N-CA-C	5.27	117.93	111.82
2	B	465	GLU	O-C-N	-5.27	117.15	123.31
2	B	538	ALA	O-C-N	-5.27	115.60	122.39
2	D	45	ARG	O-C-N	-5.27	116.44	122.08
2	B	584	ALA	CA-C-O	-5.26	114.97	120.55
2	D	171	ASP	CA-CB-CG	5.26	117.86	112.60
2	D	363	PHE	N-CA-C	5.26	117.92	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	PRO	N-CA-CB	5.26	107.99	103.36
1	A	592	GLN	CB-CA-C	-5.26	102.06	110.79
2	B	269	GLN	O-C-N	-5.26	112.88	122.34
1	C	711	ILE	O-C-N	-5.26	117.06	120.42
1	C	712	PRO	N-CA-CB	5.26	108.85	103.23
2	B	229	PRO	O-C-N	-5.25	114.99	122.35
2	B	269	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	261	ALA	O-C-N	-5.25	116.17	122.15
2	B	204	PHE	O-C-N	-5.25	116.56	122.12
1	C	480	VAL	N-CA-C	5.25	117.18	108.99
1	C	169	GLY	O-C-N	-5.24	115.89	122.70
1	A	590	PHE	CA-C-N	5.24	127.56	120.38
1	A	590	PHE	C-N-CA	5.24	127.56	120.38
1	C	18	PRO	N-CA-CB	5.24	108.75	103.25
1	C	618	ALA	CA-C-O	-5.24	115.29	120.90
2	D	101	ASN	N-CA-C	5.24	119.31	113.02
2	D	404	TYR	CB-CA-C	-5.24	102.59	110.92
1	A	422	GLY	O-C-N	-5.24	116.57	122.28
1	C	596	ARG	NE-CZ-NH2	-5.24	114.49	119.20
1	A	441	ILE	CA-C-N	5.24	124.69	119.24
1	A	441	ILE	C-N-CA	5.24	124.69	119.24
1	C	687	VAL	O-C-N	-5.24	116.49	122.62
2	D	361	LEU	CA-C-N	5.24	125.17	119.78
2	D	361	LEU	C-N-CA	5.24	125.17	119.78
1	C	23	ARG	CA-C-N	5.24	127.72	120.29
1	C	23	ARG	C-N-CA	5.24	127.72	120.29
1	C	367	SER	O-C-N	-5.24	116.09	123.11
1	A	230	ALA	CA-C-O	5.23	126.05	120.24
1	A	309	ALA	CA-C-N	5.23	127.24	120.44
1	A	309	ALA	C-N-CA	5.23	127.24	120.44
1	C	112	GLY	CA-C-O	-5.23	115.60	120.57
1	A	711	ILE	N-CA-C	5.23	119.21	112.67
2	B	183	TYR	CA-C-N	5.23	127.81	120.28
2	B	183	TYR	C-N-CA	5.23	127.81	120.28
2	B	298	ARG	CA-C-N	5.23	127.72	120.29
2	B	298	ARG	C-N-CA	5.23	127.72	120.29
1	A	66	GLY	CA-C-N	5.23	131.80	122.13
1	A	66	GLY	C-N-CA	5.23	131.80	122.13
2	D	128	GLY	CA-C-O	-5.23	115.67	120.80
1	C	371	ALA	CA-C-N	5.23	127.73	122.66
1	C	371	ALA	C-N-CA	5.23	127.73	122.66
1	A	326	ARG	O-C-N	-5.22	117.37	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	298	ARG	NH1-CZ-NH2	-5.22	112.51	119.30
2	D	254	TRP	O-C-N	-5.22	114.66	122.39
2	D	479	PHE	CA-C-N	5.22	125.22	119.89
2	D	479	PHE	C-N-CA	5.22	125.22	119.89
1	A	388	LEU	CA-C-N	5.22	127.28	120.28
1	A	388	LEU	C-N-CA	5.22	127.28	120.28
1	A	469	LYS	CA-C-N	5.22	129.77	122.36
1	A	469	LYS	C-N-CA	5.22	129.77	122.36
2	B	147	PRO	N-CA-CB	5.22	109.14	103.30
2	B	305	ALA	O-C-N	-5.22	115.85	122.27
1	C	713	GLU	O-C-N	-5.22	116.59	122.12
1	C	374	LEU	CA-C-N	5.22	125.15	119.78
1	C	374	LEU	C-N-CA	5.22	125.15	119.78
1	A	475	GLU	CA-CB-CG	5.22	124.53	114.10
2	B	170	TYR	N-CA-C	5.22	120.50	113.72
1	C	723	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	271	GLU	CA-C-N	5.21	129.42	120.72
1	A	271	GLU	C-N-CA	5.21	129.42	120.72
1	A	412	LEU	O-C-N	-5.21	116.60	122.12
1	C	380	ALA	O-C-N	-5.21	115.86	122.27
2	D	455	ASN	O-C-N	-5.21	115.18	122.37
2	B	523	ASP	O-C-N	5.21	128.47	122.17
1	C	480	VAL	CB-CA-C	-5.21	103.40	110.90
1	C	102	TYR	N-CA-C	5.20	117.63	111.33
1	C	717	SER	O-C-N	-5.20	115.87	122.27
2	D	503	ARG	O-C-N	-5.20	116.71	122.07
1	A	524	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	396	ASN	CB-CA-C	-5.20	101.58	109.89
1	C	73	GLY	N-CA-C	-5.20	101.74	112.34
1	C	330	GLN	OE1-CD-NE2	5.20	127.80	122.60
1	C	696	LEU	CA-C-O	-5.20	115.34	120.90
1	A	588	GLU	CA-C-N	5.19	127.19	120.44
1	A	588	GLU	C-N-CA	5.19	127.19	120.44
1	A	632	PRO	N-CA-CB	5.19	108.19	103.15
1	A	524	ASP	O-C-N	-5.19	114.85	122.43
2	B	218	GLY	CA-C-N	5.19	129.44	121.19
2	B	218	GLY	C-N-CA	5.19	129.44	121.19
1	C	684	VAL	CA-CB-CG2	5.19	119.23	110.40
1	A	541	ALA	O-C-N	-5.19	114.71	122.39
1	A	674	LYS	O-C-N	-5.19	116.15	122.22
2	B	452	ARG	CA-C-N	5.19	127.24	120.28
2	B	452	ARG	C-N-CA	5.19	127.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ILE	N-CA-CB	5.19	118.48	111.21
1	C	575	LYS	CA-C-N	5.19	129.73	122.36
1	C	575	LYS	C-N-CA	5.19	129.73	122.36
1	A	402	PRO	N-CA-CB	5.19	109.04	103.33
2	B	257	ALA	O-C-N	-5.19	116.73	122.07
1	A	82	ARG	CD-NE-CZ	5.19	131.66	124.40
1	A	415	ASP	CA-C-N	5.19	127.23	120.28
1	A	415	ASP	C-N-CA	5.19	127.23	120.28
1	A	190	GLU	CA-C-N	5.18	131.76	122.38
1	A	190	GLU	C-N-CA	5.18	131.76	122.38
1	C	159	ASP	CB-CG-OD1	5.18	130.33	118.40
2	D	497	PHE	CA-CB-CG	-5.18	108.62	113.80
1	C	337	THR	O-C-N	-5.18	116.42	123.10
2	D	87	TYR	CA-C-N	5.18	125.59	119.99
2	D	87	TYR	C-N-CA	5.18	125.59	119.99
2	D	110	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	A	556	PHE	N-CA-CB	-5.18	102.56	110.33
2	B	24	ALA	CB-CA-C	-5.18	99.49	110.31
2	B	27	PHE	CA-C-N	5.18	125.11	119.78
2	B	27	PHE	C-N-CA	5.18	125.11	119.78
2	B	425	LYS	O-C-N	-5.18	115.66	122.39
1	C	133	ALA	CA-C-N	5.18	133.35	121.34
1	C	133	ALA	C-N-CA	5.18	133.35	121.34
1	C	157	PRO	N-CA-CB	5.18	108.69	103.25
1	C	541	ALA	CA-C-O	5.18	125.90	119.12
1	C	586	LEU	O-C-N	-5.18	116.63	122.12
1	C	360	THR	CA-C-O	5.17	127.87	121.87
1	A	123	ARG	CA-C-N	5.17	129.79	121.00
1	A	123	ARG	C-N-CA	5.17	129.79	121.00
1	A	220	ILE	CA-CB-CG2	5.17	119.29	110.50
2	B	413	ALA	CA-C-N	5.17	127.20	120.28
2	B	413	ALA	C-N-CA	5.17	127.20	120.28
1	C	278	ASP	CB-CG-OD1	5.17	130.29	118.40
1	C	314	GLN	CA-CB-CG	5.17	124.44	114.10
1	A	359	HIS	ND1-CE1-NE2	5.17	113.57	108.40
1	A	585	GLU	CA-C-O	-5.17	115.37	120.90
1	A	339	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	C	493	LYS	O-C-N	-5.16	116.75	122.07
1	A	26	GLU	CA-C-O	-5.16	115.06	120.63
1	A	359	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
2	B	268	GLU	N-CA-CB	5.16	117.70	110.12
2	B	410	ARG	CA-C-N	5.16	127.19	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	ARG	C-N-CA	5.16	127.19	120.28
2	B	531	SER	CA-C-O	5.16	125.96	120.24
1	C	319	ASN	O-C-N	-5.15	115.64	121.36
2	D	146	ALA	CA-C-O	5.15	126.51	120.69
2	B	540	ILE	CA-C-O	-5.15	114.97	120.59
1	C	678	PRO	O-C-N	-5.15	115.31	122.37
1	A	49	LEU	CA-C-O	5.15	126.42	120.14
2	B	62	LEU	N-CA-CB	-5.15	102.56	110.44
2	D	301	ARG	CA-C-N	5.15	127.49	120.54
2	D	301	ARG	C-N-CA	5.15	127.49	120.54
1	C	179	VAL	CA-C-N	5.15	127.73	120.42
1	C	179	VAL	C-N-CA	5.15	127.73	120.42
1	C	642	ARG	CD-NE-CZ	5.14	131.60	124.40
2	B	141	ASP	CA-CB-CG	5.14	117.74	112.60
2	D	355	ALA	CA-C-O	5.14	126.92	121.16
2	B	228	SER	CA-C-O	5.14	127.20	120.16
2	B	398	PRO	O-C-N	-5.14	115.35	122.24
1	C	184	GLU	O-C-N	-5.14	115.59	122.43
1	A	208	ASN	OD1-CG-ND2	5.14	127.74	122.60
2	D	97	THR	CA-CB-CG2	5.14	119.23	110.50
1	C	280	PHE	O-C-N	-5.14	115.76	122.59
2	D	212	PRO	N-CA-CB	5.14	107.41	103.30
1	A	207	ARG	O-C-N	-5.13	115.42	122.46
2	B	432	ALA	O-C-N	-5.13	116.78	122.07
1	C	334	TRP	O-C-N	-5.13	116.68	122.12
1	C	438	GLU	CB-CG-CD	5.13	121.33	112.60
1	C	677	ARG	CA-C-N	5.13	125.58	120.04
1	C	677	ARG	C-N-CA	5.13	125.58	120.04
1	C	176	ALA	N-CA-C	5.13	116.88	111.28
1	A	654	VAL	O-C-N	5.13	128.51	122.81
1	C	172	LEU	CA-C-N	5.13	124.31	118.97
1	C	172	LEU	C-N-CA	5.13	124.31	118.97
2	D	150	LEU	CA-C-N	5.13	127.47	120.54
2	D	150	LEU	C-N-CA	5.13	127.47	120.54
1	A	42	GLU	CA-C-O	5.13	125.67	119.11
1	A	63	THR	N-CA-C	-5.13	102.31	109.69
1	A	465	ILE	O-C-N	-5.13	117.44	122.67
1	A	509	LYS	CA-C-N	5.13	127.57	120.29
1	A	509	LYS	C-N-CA	5.13	127.57	120.29
2	D	471	ALA	CA-C-N	5.12	128.05	120.82
2	D	471	ALA	C-N-CA	5.12	128.05	120.82
1	A	561	ALA	CA-C-O	-5.12	115.77	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	VAL	CA-CB-CG2	5.12	119.11	110.40
2	B	127	GLU	O-C-N	-5.12	116.69	122.12
1	C	63	THR	O-C-N	-5.12	115.85	122.97
2	D	20	THR	CA-C-N	-5.12	114.18	121.50
2	D	20	THR	C-N-CA	-5.12	114.18	121.50
2	D	37	ARG	O-C-N	-5.12	116.23	122.22
2	D	490	TRP	O-C-N	-5.12	117.23	123.27
2	D	531	SER	CA-CB-OG	-5.12	100.87	111.10
1	A	213	PRO	CA-C-N	5.12	126.23	119.84
1	A	213	PRO	C-N-CA	5.12	126.23	119.84
2	D	301	ARG	O-C-N	-5.12	116.77	122.09
1	A	660	GLY	O-C-N	-5.11	116.44	122.27
2	D	512	LYS	CB-CA-C	-5.11	98.22	109.56
1	C	17	VAL	CA-C-O	5.11	126.80	119.95
1	A	514	LYS	O-C-N	-5.11	116.71	122.12
1	C	106	LEU	O-C-N	-5.11	116.33	122.15
1	C	188	LYS	CA-C-N	5.11	124.90	119.28
1	C	188	LYS	C-N-CA	5.11	124.90	119.28
1	A	70	PHE	CB-CA-C	-5.10	104.35	111.80
1	A	722	LEU	CA-C-N	5.10	127.07	120.44
1	A	722	LEU	C-N-CA	5.10	127.07	120.44
2	B	489	ALA	CA-C-N	5.10	130.36	123.11
2	B	489	ALA	C-N-CA	5.10	130.36	123.11
1	C	435	LYS	O-C-N	-5.10	116.71	122.12
1	C	177	LEU	O-C-N	-5.10	116.25	122.22
1	A	673	ASP	CA-CB-CG	5.10	117.70	112.60
2	D	58	CYS	O-C-N	-5.10	116.34	122.15
2	D	328	TRP	N-CA-C	-5.10	105.36	112.45
2	B	282	PHE	CA-C-O	-5.09	114.86	120.36
2	B	533	PRO	O-C-N	-5.09	116.12	122.23
2	D	257	ALA	CA-C-N	5.09	127.62	120.28
2	D	257	ALA	C-N-CA	5.09	127.62	120.28
1	A	643	GLN	O-C-N	-5.09	116.34	122.15
1	A	719	VAL	O-C-N	-5.09	116.85	121.94
2	B	31	THR	CA-CB-CG2	5.09	119.16	110.50
2	B	247	GLY	N-CA-C	-5.09	103.59	112.55
1	C	281	ALA	N-CA-CB	5.09	118.32	110.43
1	A	268	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	C	599	ARG	CA-C-N	-5.09	115.87	122.94
1	C	599	ARG	C-N-CA	-5.09	115.87	122.94
1	C	669	ARG	NE-CZ-NH1	5.08	126.58	121.50
2	B	541	ASP	N-CA-CB	5.08	117.53	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ALA	N-CA-CB	-5.08	102.65	110.12
2	D	440	LYS	N-CA-C	5.08	116.51	111.07
1	A	232	MET	CA-CB-CG	5.08	124.27	114.10
1	A	416	LEU	O-C-N	-5.08	116.73	122.12
1	C	479	ASP	O-C-N	-5.08	115.91	122.77
2	B	78	PRO	CA-C-N	5.08	130.44	120.99
2	B	78	PRO	C-N-CA	5.08	130.44	120.99
1	C	524	ASP	O-C-N	-5.08	115.63	122.43
1	C	104	ARG	CG-CD-NE	5.08	123.17	112.00
1	C	289	GLY	O-C-N	-5.07	117.12	123.21
2	D	615	GLY	CA-C-O	-5.07	116.65	121.62
1	C	243	TYR	CB-CG-CD2	5.07	128.41	120.80
1	A	20	ASP	CA-C-O	5.07	125.81	119.78
2	B	462	ALA	O-C-N	-5.07	113.87	122.03
2	D	180	VAL	N-CA-CB	5.07	118.19	110.58
1	A	283	ARG	CB-CA-C	5.07	118.55	110.09
1	A	400	ILE	CA-C-O	5.07	126.72	120.74
2	B	229	PRO	N-CA-CB	5.07	108.17	103.41
2	B	240	ILE	CA-C-O	-5.07	115.80	121.17
1	C	100	ALA	CA-C-N	5.07	127.32	120.38
1	C	100	ALA	C-N-CA	5.07	127.32	120.38
2	D	478	PRO	N-CA-CB	5.07	107.71	103.25
1	A	719	VAL	CA-C-N	5.06	127.07	120.28
1	A	719	VAL	C-N-CA	5.06	127.07	120.28
1	C	376	THR	N-CA-C	-5.06	102.51	110.36
2	D	351	SER	O-C-N	-5.06	116.38	122.15
2	B	610	GLU	O-C-N	-5.06	116.75	122.12
1	C	462	GLN	OE1-CD-NE2	5.06	127.66	122.60
1	C	666	PRO	O-C-N	-5.06	116.16	122.23
2	D	422	GLU	CA-C-N	5.06	127.60	120.42
2	D	422	GLU	C-N-CA	5.06	127.60	120.42
2	B	176	ALA	CA-C-N	5.05	127.81	120.79
2	B	176	ALA	C-N-CA	5.05	127.81	120.79
2	B	233	ALA	CA-C-O	5.05	125.96	120.55
2	D	422	GLU	N-CA-C	5.05	118.22	111.75
1	C	366	ASN	N-CA-CB	5.05	117.30	110.38
1	C	521	ASN	O-C-N	-5.05	116.84	121.34
1	C	554	LYS	CA-C-O	-5.05	115.18	120.63
2	D	450	ALA	CA-C-N	5.05	127.32	120.65
2	D	450	ALA	C-N-CA	5.05	127.32	120.65
1	C	30	ALA	O-C-N	-5.05	116.39	122.15
2	D	154	LEU	CA-C-N	5.05	127.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	154	LEU	C-N-CA	5.05	127.55	120.28
2	D	352	VAL	CA-C-N	5.05	132.44	121.19
2	D	352	VAL	C-N-CA	5.05	132.44	121.19
2	D	299	ALA	CA-C-O	-5.04	115.20	120.55
2	D	637	ALA	CA-C-O	5.04	127.72	120.51
2	B	353	GLY	CA-C-N	5.04	129.57	121.00
2	B	353	GLY	C-N-CA	5.04	129.57	121.00
1	C	206	VAL	CB-CA-C	-5.04	103.02	111.29
1	A	49	LEU	CB-CA-C	-5.04	101.38	109.89
2	B	442	LEU	CA-C-N	5.04	127.97	120.31
2	B	442	LEU	C-N-CA	5.04	127.97	120.31
1	C	93	SER	N-CA-CB	-5.04	101.98	110.49
1	C	130	PRO	O-C-N	-5.04	115.72	122.22
2	B	200	ASP	CA-C-O	5.04	127.06	120.16
2	B	329	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	25	PHE	N-CA-CB	5.04	117.31	110.01
2	D	347	THR	CA-C-O	5.04	125.89	120.55
2	D	364	THR	CB-CA-C	-5.04	100.50	110.27
2	B	66	THR	CA-C-N	5.03	127.63	120.53
2	B	66	THR	C-N-CA	5.03	127.63	120.53
1	A	78	MET	CA-C-O	5.03	127.70	120.51
1	A	339	GLN	CA-C-N	5.03	130.43	122.78
1	A	339	GLN	C-N-CA	5.03	130.43	122.78
1	C	691	GLN	CG-CD-OE1	-5.03	110.74	120.80
2	B	393	GLY	CA-C-N	5.03	127.95	120.31
2	B	393	GLY	C-N-CA	5.03	127.95	120.31
2	B	492	ARG	CD-NE-CZ	5.03	131.44	124.40
1	C	726	LEU	CA-C-O	5.03	125.72	119.79
2	D	274	THR	CA-C-O	-5.03	115.54	120.82
1	C	79	TYR	O-C-N	-5.03	115.09	122.43
1	A	176	ALA	O-C-N	-5.03	116.42	122.15
1	A	328	HIS	N-CA-C	-5.03	103.08	110.52
1	C	404	SER	CB-CA-C	-5.02	103.08	110.06
2	D	127	GLU	CA-C-O	5.02	127.69	120.51
1	A	29	ALA	O-C-N	-5.02	116.80	122.12
1	A	54	VAL	O-C-N	-5.02	116.80	121.87
1	C	515	ILE	O-C-N	-5.02	116.77	121.94
1	C	398	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	C	710	VAL	N-CA-CB	-5.02	105.25	110.72
1	C	74	PRO	N-CA-CB	5.01	108.83	103.52
2	D	17	THR	CA-C-N	5.01	124.91	119.85
2	D	17	THR	C-N-CA	5.01	124.91	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	ALA	CA-C-O	-5.01	115.21	120.92
2	B	115	ASP	CA-C-N	5.01	124.61	119.05
2	B	115	ASP	C-N-CA	5.01	124.61	119.05
1	C	179	VAL	O-C-N	-5.01	117.02	121.87
1	A	321	LYS	CA-C-N	5.00	126.98	120.28
1	A	321	LYS	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	MET	Mainchain
1	A	194	GLY	Mainchain
1	A	231	ASN	Mainchain
1	A	268	ARG	Mainchain
1	A	277	VAL	Mainchain
1	A	278	ASP	Mainchain
1	A	280	PHE	Mainchain
1	A	281	ALA	Mainchain
1	A	342	TYR	Mainchain
1	A	371	ALA	Mainchain
1	A	376	THR	Mainchain
1	A	394	SER	Mainchain
1	A	395	GLY	Mainchain
1	A	40	THR	Mainchain
1	A	405	GLY	Mainchain
1	A	41	ALA	Mainchain
1	A	420	ALA	Mainchain
1	A	504	ASP	Mainchain
1	A	540	ARG	Mainchain
1	A	61	LEU	Mainchain
1	A	633	LEU	Mainchain
1	A	645	VAL	Mainchain
1	A	670	LYS	Mainchain
1	A	70	PHE	Mainchain
1	A	87	ARG	Mainchain
2	B	106	ALA	Mainchain
2	B	129	LEU	Mainchain
2	B	154	LEU	Mainchain
2	B	173	GLY	Mainchain
2	B	222	ARG	Mainchain
2	B	246	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	B	264	ARG	Mainchain
2	B	273	ALA	Mainchain
2	B	334	GLU	Mainchain
2	B	394	ARG	Mainchain
2	B	401	GLY	Mainchain
2	B	456	ARG	Mainchain
2	B	457	LYS	Mainchain
2	B	500	LEU	Mainchain
2	B	521	ARG	Mainchain
2	B	522	ARG	Mainchain
2	B	599	PHE	Mainchain
2	B	629	SER	Mainchain
2	B	71	ASP	Mainchain
2	B	84	LYS	Mainchain
2	B	86	GLY	Mainchain
1	C	162	SER	Mainchain
1	C	167	MET	Mainchain
1	C	179	VAL	Mainchain
1	C	183	GLU	Mainchain
1	C	194	GLY	Mainchain
1	C	205	MET	Mainchain
1	C	228	THR	Mainchain
1	C	230	ALA	Mainchain
1	C	268	ARG	Mainchain
1	C	271	GLU	Mainchain
1	C	285	SER	Mainchain
1	C	292	MET	Mainchain
1	C	357	GLN	Mainchain
1	C	359	HIS	Mainchain
1	C	369	ASP	Mainchain
1	C	371	ALA	Mainchain
1	C	376	THR	Mainchain
1	C	391	GLN	Mainchain
1	C	394	SER	Mainchain
1	C	40	THR	Mainchain
1	C	403	TRP	Mainchain
1	C	405	GLY	Mainchain
1	C	460	GLY	Mainchain
1	C	479	ASP	Mainchain
1	C	51	ASN	Mainchain
1	C	526	ASP	Mainchain
1	C	531	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	C	540	ARG	Mainchain
1	C	588	GLU	Mainchain
1	C	622	ALA	Mainchain
1	C	638	GLU	Mainchain
1	C	645	VAL	Mainchain
1	C	674	LYS	Mainchain
1	C	677	ARG	Mainchain
1	C	693	PHE	Mainchain
1	C	70	PHE	Mainchain
1	C	723	ARG	Mainchain
2	D	154	LEU	Mainchain
2	D	220	TRP	Mainchain
2	D	228	SER	Mainchain
2	D	287	THR	Mainchain
2	D	319	GLY	Mainchain
2	D	334	GLU	Mainchain
2	D	335	ASP	Mainchain
2	D	336	PRO	Mainchain
2	D	338	VAL	Mainchain
2	D	348	PHE	Mainchain
2	D	35	TRP	Mainchain
2	D	401	GLY	Mainchain
2	D	456	ARG	Mainchain
2	D	563	GLN	Mainchain
2	D	61	ARG	Mainchain
2	D	622	ASP	Mainchain
2	D	86	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5563	0	5443	41	0
1	C	5560	0	5456	53	0
2	B	4695	0	4610	45	0
2	D	4692	0	4580	53	0
3	A	91	0	88	13	0
3	C	91	0	88	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	12	0	16	3	0
5	B	18	0	24	2	0
5	C	12	0	16	3	0
5	D	12	0	15	1	0
6	A	457	0	0	0	0
6	B	318	0	0	1	0
6	C	493	0	0	2	0
6	D	264	0	0	0	0
All	All	22372	0	20400	195	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 (195) 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:A:800:B12:H421	3:A:800:B12:C36	1.67	1.23
3:A:800:B12:H421	3:A:800:B12:H363	1.18	1.12
3:A:800:B12:H552	3:A:800:B12:H531	1.24	1.10
3:A:800:B12:H363	3:A:800:B12:C42	1.93	0.96
3:A:800:B12:C36	3:A:800:B12:C42	2.36	0.90
3:A:800:B12:H351	3:A:800:B12:H372	1.51	0.90
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.20	0.89
1:C:330:GLN:HE22	5:C:802:GOL:H31	1.39	0.88
3:A:800:B12:H421	3:A:800:B12:H361	1.57	0.86
3:A:800:B12:H531	3:A:800:B12:C55	2.02	0.84
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.25	0.83
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.62	0.80
3:C:800:B12:H372	3:C:800:B12:H351	1.64	0.80
2:B:468:MET:HE3	2:B:471:ALA:HA	1.70	0.74
1:A:330:GLN:HE22	5:A:802:GOL:H31	1.53	0.73
1:C:638:GLU:HA	1:C:671:GLU:HG3	1.70	0.72
3:C:800:B12:H531	3:C:800:B12:H552	1.71	0.72
1:A:24:ARG:HH22	2:B:315:GLU:HG3	1.57	0.70
2:D:180:VAL:HG13	2:D:197:LEU:HD21	1.72	0.69
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.75	0.68
2:D:83:LYS:H	2:D:84:LYS:HZ2	1.41	0.68
2:B:586:LYS:HD3	2:B:593:LEU:HD12	1.74	0.68
3:C:800:B12:H203	3:C:800:B12:H301	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:617:LEU:HD22	2:B:621:MET:HE1	1.76	0.65
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.79	0.65
3:A:800:B12:H372	3:A:800:B12:C35	2.26	0.65
1:C:247:GLU:HB3	3:C:800:B12:H532	1.78	0.64
1:C:374:LEU:HB2	1:C:481:LEU:HD23	1.78	0.64
1:C:706:THR:HB	1:C:707:PRO:CD	2.27	0.64
1:A:247:GLU:HB3	3:A:800:B12:H532	1.78	0.64
1:A:706:THR:HB	1:A:707:PRO:HD2	1.79	0.64
2:B:98:THR:HB	5:B:639:GOL:H11	1.80	0.63
1:A:359:HIS:CE1	1:A:401:ASP:H	2.16	0.63
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.81	0.63
2:D:83:LYS:H	2:D:84:LYS:NZ	1.96	0.62
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.45	0.62
1:C:188:LYS:H	1:C:191:GLN:HE21	1.48	0.61
1:C:188:LYS:H	1:C:191:GLN:NE2	1.98	0.61
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.83	0.61
1:A:188:LYS:H	1:A:191:GLN:HE21	1.49	0.61
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.48	0.61
2:D:191:LYS:HA	2:D:227:PHE:HA	1.82	0.61
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.84	0.60
2:B:391:ASN:ND2	2:B:394:ARG:HE	2.01	0.58
2:D:108:ASP:HB3	2:D:357:SER:HA	1.85	0.58
1:A:706:THR:HB	1:A:707:PRO:CD	2.33	0.58
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.85	0.58
1:C:706:THR:HB	1:C:707:PRO:HD2	1.85	0.57
1:A:139:ALA:HB1	3:A:800:B12:H362	1.85	0.57
1:C:330:GLN:NE2	5:C:802:GOL:H31	2.16	0.57
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.87	0.57
1:A:188:LYS:H	1:A:191:GLN:NE2	2.02	0.56
2:D:138:LEU:HD23	2:D:145:ILE:HD13	1.88	0.56
1:A:374:LEU:HB2	1:A:481:LEU:HD23	1.87	0.56
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.88	0.56
1:C:357:GLN:HE22	2:D:290:GLN:NE2	2.01	0.56
3:C:800:B12:H372	3:C:800:B12:C35	2.36	0.56
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.87	0.55
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.89	0.55
2:D:172:GLN:NE2	2:D:204:PHE:HB2	2.21	0.54
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.05	0.54
2:D:297:LEU:HA	2:D:322:GLN:HE22	1.72	0.54
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.55	0.54
1:C:359:HIS:CE1	1:C:401:ASP:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:THR:HG22	1:A:580:VAL:H	1.72	0.54
2:B:493:ASP:HA	5:B:640:GOL:H31	1.90	0.53
3:A:800:B12:H601	3:A:800:B12:H252	1.91	0.53
1:A:651:VAL:HB	1:A:722:LEU:HD21	1.91	0.52
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.92	0.52
1:A:359:HIS:HE1	1:A:401:ASP:H	1.57	0.52
1:C:571:SER:HB3	1:C:623:ASP:HB3	1.91	0.52
1:A:357:GLN:HE22	2:B:290:GLN:NE2	2.00	0.52
1:C:602:LEU:HD12	1:C:618:ALA:HB2	1.92	0.51
1:C:372:ILE:HG22	1:C:480:VAL:HG11	1.91	0.51
1:A:683:THR:HG21	1:A:718:LEU:HD13	1.94	0.50
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.93	0.50
2:D:212:PRO:HD2	2:D:434:MET:HE2	1.92	0.50
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.94	0.50
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.58	0.50
2:B:579:LEU:HD11	2:B:583:LYS:HE3	1.92	0.50
1:A:133:ALA:HB1	1:A:489:LEU:HD21	1.93	0.50
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.93	0.50
1:C:372:ILE:HG23	6:C:1277:HOH:O	2.12	0.50
1:C:372:ILE:CG2	1:C:480:VAL:HG11	2.41	0.49
3:C:800:B12:H531	3:C:800:B12:C55	2.40	0.49
2:D:532:SER:CB	2:D:533:PRO:HD3	2.43	0.49
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.94	0.49
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.95	0.49
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.37	0.49
2:B:202:ILE:HG13	2:B:214:LEU:HD11	1.94	0.49
2:D:122:ARG:HB3	2:D:122:ARG:HH11	1.77	0.49
3:C:800:B12:C47	3:C:800:B12:H492	2.43	0.49
1:C:7:PHE:HA	1:C:10:VAL:HG23	1.95	0.48
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.95	0.48
1:A:149:MET:HG3	1:A:177:LEU:HB3	1.94	0.48
1:A:330:GLN:NE2	5:A:802:GOL:H31	2.26	0.48
2:B:468:MET:HE1	6:B:646:HOH:O	2.14	0.48
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.94	0.47
1:C:15:ALA:HA	1:C:16:PRO:HD2	1.57	0.47
2:B:503:ARG:NE	2:B:638:LYS:HB3	2.30	0.47
2:B:284:VAL:HG11	2:B:322:GLN:HE21	1.79	0.47
1:C:69:PRO:HB2	1:C:306:MET:HG2	1.96	0.47
1:C:94:THR:HG22	1:C:488:VAL:HG13	1.97	0.46
2:D:468:MET:HE3	2:D:471:ALA:HA	1.98	0.46
1:C:149:MET:HG3	1:C:177:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.96	0.46
2:D:234:VAL:HB	2:D:280:ILE:HG12	1.97	0.46
1:A:541:ALA:O	1:A:542:MET:HB2	2.15	0.46
1:C:15:ALA:HB1	2:D:92:PRO:HG3	1.98	0.46
1:C:52:GLU:HG3	2:D:85:LEU:HG	1.97	0.46
2:D:83:LYS:HB2	2:D:84:LYS:HZ1	1.81	0.45
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.98	0.45
1:C:44:ILE:HD11	1:C:419:LYS:HD2	1.98	0.45
1:C:54:VAL:O	1:C:58:MET:HE3	2.17	0.45
2:D:107:TRP:CD1	2:D:358:ILE:HD12	2.51	0.45
2:B:80:ASP:HB3	2:B:407:SER:HB2	1.97	0.45
2:B:431:LYS:O	2:B:435:THR:HB	2.16	0.45
1:A:310:LYS:HE2	2:B:21:LEU:HD11	1.98	0.45
1:A:606:GLY:O	1:A:634:PHE:HA	2.16	0.45
1:A:599:ARG:HG2	1:A:649:VAL:HA	1.99	0.45
1:C:215:GLN:N	1:C:216:PRO:HD2	2.31	0.45
1:C:415:ASP:O	1:C:419:LYS:HG3	2.17	0.45
2:B:116:PRO:HG3	2:B:480:PRO:HG3	1.99	0.45
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.51	0.45
1:C:305:ARG:HG2	1:C:325:LEU:HB3	1.99	0.45
1:C:458:ASP:HB3	1:C:710:VAL:HG13	1.99	0.45
3:C:800:B12:HM63	3:C:800:B12:HM51	1.80	0.45
1:A:485:ASN:O	1:A:486:SER:C	2.60	0.44
1:A:188:LYS:N	1:A:191:GLN:HE21	2.12	0.44
1:C:17:VAL:N	2:D:92:PRO:HD3	2.32	0.44
1:C:197:GLN:HA	1:C:239:SER:HB3	1.99	0.44
1:C:14:ASN:O	1:C:15:ALA:C	2.60	0.44
1:C:358:GLY:O	1:C:359:HIS:HB2	2.17	0.44
2:D:397:ASP:N	2:D:398:PRO:HD3	2.32	0.44
1:A:372:ILE:HG22	1:A:480:VAL:HG11	2.00	0.44
1:A:514:LYS:HD3	1:A:534:LEU:HD22	2.00	0.44
1:C:139:ALA:HB1	3:C:800:B12:H362	1.99	0.44
2:D:113:HIS:HB2	2:D:138:LEU:HG	2.00	0.44
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.99	0.44
1:C:484:ASP:O	1:C:485:ASN:C	2.60	0.44
2:D:252:LEU:HD11	2:D:300:LEU:HA	1.99	0.44
1:A:69:PRO:HG3	2:B:24:ALA:HA	2.01	0.43
2:B:518:LEU:HB2	2:B:569:SER:HB2	2.00	0.43
1:C:711:ILE:N	1:C:712:PRO:HD2	2.33	0.43
1:A:129:ASN:HA	1:A:130:PRO:HD2	1.88	0.43
2:D:370:PRO:HB3	2:D:375:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:GLY:O	2:D:222:ARG:HG3	2.18	0.43
2:D:365:GLN:HE21	5:D:1:GOL:H31	1.83	0.43
1:A:4:LEU:HD13	2:B:264:ARG:HG2	2.01	0.43
1:A:4:LEU:HA	1:A:5:PRO:HD2	1.89	0.43
2:D:390:VAL:HG12	2:D:392:ILE:HG23	2.00	0.43
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.54	0.43
2:B:193:LEU:O	2:B:227:PHE:HB3	2.19	0.43
1:C:605:MET:HE3	1:C:664:LEU:HB3	2.00	0.43
2:D:429:MET:HA	2:D:432:ALA:HB3	2.01	0.43
1:C:6:ARG:HD3	1:C:6:ARG:HA	1.89	0.42
2:B:331:LEU:HD13	2:B:365:GLN:HB3	2.01	0.42
1:C:330:GLN:HE22	5:C:802:GOL:C3	2.21	0.42
2:D:146:ALA:HB3	2:D:149:HIS:ND1	2.34	0.42
2:B:114:GLU:HG2	2:B:139:ARG:HB2	2.01	0.42
2:B:334:GLU:O	2:B:335:ASP:C	2.62	0.42
2:B:274:THR:HA	2:B:313:VAL:HG13	2.01	0.42
1:C:641:ALA:CB	1:C:671:GLU:HB3	2.49	0.42
1:C:521:ASN:O	1:C:529:ARG:HD3	2.20	0.42
2:D:294:ILE:HG12	2:D:352:VAL:HB	2.02	0.42
2:D:334:GLU:O	2:D:335:ASP:C	2.62	0.42
2:D:517:CYS:HB2	2:D:545:VAL:O	2.20	0.42
3:A:800:B12:H361	3:A:800:B12:H412	1.84	0.42
2:B:468:MET:HE2	2:B:468:MET:HB3	1.87	0.42
2:D:267:VAL:HA	2:D:271:PHE:O	2.20	0.41
1:A:281:ALA:HA	1:A:284:LEU:HG	2.01	0.41
1:A:116:ALA:O	1:A:141:VAL:HG12	2.20	0.41
2:D:80:ASP:HB3	2:D:407:SER:HB2	2.02	0.41
2:B:115:ASP:OD2	2:B:477:LYS:HE3	2.21	0.41
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.49	0.41
2:D:83:LYS:N	2:D:84:LYS:HZ2	2.14	0.41
1:A:203:GLU:HA	1:A:207:ARG:HB3	2.02	0.41
2:D:125:ILE:HD11	2:D:138:LEU:HD21	2.02	0.41
2:D:263:VAL:O	2:D:267:VAL:HG23	2.20	0.41
2:B:369:LEU:O	2:B:370:PRO:C	2.64	0.41
1:C:16:PRO:HD2	2:D:92:PRO:HB3	2.01	0.41
1:A:246:GLN:HE22	1:A:291:GLY:HA3	1.86	0.41
2:D:532:SER:HB3	2:D:533:PRO:HD3	2.02	0.41
1:C:252:ALA:O	1:C:256:MET:HG3	2.21	0.41
1:C:563:ILE:HD11	6:C:1048:HOH:O	2.21	0.41
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.51	0.41
2:D:455:ASN:HA	2:D:621:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TYR:HE2	5:A:802:GOL:H2	1.86	0.40
3:C:800:B12:H203	3:C:800:B12:C30	2.47	0.40
2:D:81:ALA:O	2:D:82:PRO:C	2.64	0.40
1:C:386:THR:HA	2:D:341:LEU:HD13	2.02	0.40
1:A:10:VAL:HG11	2:B:310:VAL:HG21	2.03	0.40
2:D:369:LEU:O	2:D:370:PRO:C	2.65	0.40
2:D:571:ALA:HA	2:D:601:GLU:HB3	2.03	0.40
2:B:589:GLY:O	2:B:590:ALA:C	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/727 (100%)	698 (96%)	26 (4%)	1 (0%)	48	46
1	C	725/727 (100%)	685 (94%)	37 (5%)	3 (0%)	30	27
2	B	617/637 (97%)	595 (96%)	21 (3%)	1 (0%)	43	42
2	D	620/637 (97%)	580 (94%)	38 (6%)	2 (0%)	36	35
All	All	2687/2728 (98%)	2558 (95%)	122 (4%)	7 (0%)	36	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ALA
1	C	16	PRO
2	D	228	SER
1	A	486	SER
1	C	486	SER
2	B	45	ARG
2	D	435	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/590 (97%)	550 (96%)	21 (4%)	30	30
1	C	571/590 (97%)	549 (96%)	22 (4%)	28	28
2	B	474/509 (93%)	455 (96%)	19 (4%)	28	27
2	D	472/509 (93%)	449 (95%)	23 (5%)	22	20
All	All	2088/2198 (95%)	2003 (96%)	85 (4%)	27	26

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	LEU
1	A	9	SER
1	A	93	SER
1	A	127	SER
1	A	202	LYS
1	A	207	ARG
1	A	430	VAL
1	A	441	ILE
1	A	473	GLU
1	A	485	ASN
1	A	567	SER
1	A	576	ASN
1	A	577	THR
1	A	585	GLU
1	A	597	ARG
1	A	599	ARG
1	A	668	LEU
1	A	669	ARG
1	A	713	GLU
1	A	725	SER
2	B	60	LYS
2	B	83	LYS
2	B	119	LYS

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Mol	Chain	Res	Type
2	B	134	THR
2	B	180	VAL
2	B	186	SER
2	B	191	LYS
2	B	216	VAL
2	B	224	LEU
2	B	226	LYS
2	B	279	THR
2	B	334	GLU
2	B	410	ARG
2	B	435	THR
2	B	436	GLU
2	B	475	GLU
2	B	586	LYS
2	B	593	LEU
2	B	629	SER
1	C	4	LEU
1	C	9	SER
1	C	52	GLU
1	C	96	LYS
1	C	202	LYS
1	C	207	ARG
1	C	419	LYS
1	C	444	MET
1	C	487	THR
1	C	488	VAL
1	C	509	LYS
1	C	558	ARG
1	C	562	GLN
1	C	567	SER
1	C	575	LYS
1	C	577	THR
1	C	589	GLU
1	C	596	ARG
1	C	668	LEU
1	C	671	GLU
1	C	691	GLN
1	C	721	LYS
2	D	83	LYS
2	D	84	LYS
2	D	122	ARG
2	D	141	ASP

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Mol	Chain	Res	Type
2	D	155	SER
2	D	185	ARG
2	D	187	ASP
2	D	227	PHE
2	D	232	ARG
2	D	297	LEU
2	D	316	ASP
2	D	317	LYS
2	D	334	GLU
2	D	371	GLU
2	D	380	ARG
2	D	410	ARG
2	D	411	SER
2	D	425	LYS
2	D	477	LYS
2	D	522	ARG
2	D	532	SER
2	D	559	LYS
2	D	617	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	160	GLN
1	A	191	GLN
1	A	246	GLN
1	A	330	GLN
1	A	359	HIS
1	A	366	ASN
1	A	385	ASN
1	A	521	ASN
1	A	592	GLN
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	365	GLN
2	B	391	ASN
2	B	577	GLN
1	C	14	ASN
1	C	191	GLN
1	C	198	ASN

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Mol	Chain	Res	Type
1	C	359	HIS
1	C	385	ASN
1	C	454	GLN
1	C	492	GLN
1	C	562	GLN
1	C	643	GLN
2	D	290	GLN
2	D	323	ASN
2	D	365	GLN
2	D	391	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
5	GOL	A	802	-	5,5,5	0.79	0	5,5,5	1.76	1 (20%)
5	GOL	B	640	-	5,5,5	0.44	0	5,5,5	0.45	0
5	GOL	C	802	-	5,5,5	1.09	0	5,5,5	2.93	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	D	1	-	5,5,5	0.61	0	5,5,5	2.14	1 (20%)
5	GOL	D	639	-	5,5,5	0.21	0	5,5,5	0.91	0
4	DCA	C	801	-	47,49,49	1.32	7 (14%)	69,74,74	1.50	13 (18%)
3	B12	A	800	1	94,101,101	1.61	19 (20%)	149,166,166	2.34	48 (32%)
4	DCA	A	801	-	47,49,49	1.64	4 (8%)	69,74,74	1.14	5 (7%)
5	GOL	A	803	-	5,5,5	0.82	0	5,5,5	0.66	0
3	B12	C	800	6,1	94,101,101	1.59	19 (20%)	149,166,166	2.58	59 (39%)
5	GOL	C	803	-	5,5,5	0.52	0	5,5,5	0.61	0
5	GOL	B	639	-	5,5,5	0.31	0	5,5,5	0.58	0
5	GOL	B	1	-	5,5,5	0.66	0	5,5,5	0.24	0

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
5	GOL	A	802	-	-	0/4/4/4	-
5	GOL	B	640	-	-	4/4/4/4	-
5	GOL	C	802	-	-	0/4/4/4	-
5	GOL	D	1	-	-	3/4/4/4	-
5	GOL	D	639	-	-	2/4/4/4	-
4	DCA	C	801	-	-	2/47/63/63	0/3/3/3
3	B12	A	800	1	-	12/56/223/223	0/3/11/11
4	DCA	A	801	-	-	2/47/63/63	0/3/3/3
5	GOL	A	803	-	-	0/4/4/4	-
3	B12	C	800	6,1	-	10/56/223/223	0/3/11/11
5	GOL	C	803	-	-	0/4/4/4	-
5	GOL	B	639	-	-	2/4/4/4	-
5	GOL	B	1	-	-	0/4/4/4	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C14-N23	7.91	1.45	1.35
4	A	801	DCA	P1A-O3A	-6.76	1.52	1.59
3	C	800	B12	C14-N23	5.38	1.42	1.35
4	A	801	DCA	P3B-O3B	4.95	1.68	1.59
4	A	801	DCA	P2A-O3A	4.26	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	C19-N24	-3.76	1.44	1.49
3	A	800	B12	P-O2	3.47	1.69	1.59
3	C	800	B12	C30-C3	3.38	1.62	1.54
3	C	800	B12	P-O2	3.34	1.69	1.59
3	C	800	B12	C12-C11	-3.26	1.46	1.52
3	A	800	B12	C2B-N1B	-3.21	1.32	1.37
3	C	800	B12	C8-C9	3.18	1.58	1.51
3	A	800	B12	C55-C56	3.18	1.60	1.53
3	C	800	B12	C48-C13	2.99	1.61	1.54
3	A	800	B12	C46-C12	2.99	1.60	1.54
4	C	801	DCA	P3B-O3B	2.95	1.64	1.59
3	A	800	B12	C41-C8	2.90	1.61	1.54
3	A	800	B12	C13-C14	-2.78	1.47	1.52
3	A	800	B12	C19-N24	-2.77	1.45	1.49
3	C	800	B12	C41-C8	2.75	1.60	1.54
3	C	800	B12	CO-N22	2.68	2.08	1.96
3	C	800	B12	C3R-C4R	2.67	1.59	1.52
4	C	801	DCA	O5P-C5P	2.58	1.28	1.23
4	C	801	DCA	C7P-N8P	2.56	1.51	1.46
3	A	800	B12	C17-C18	-2.55	1.50	1.54
4	C	801	DCA	P1A-O1A	-2.48	1.42	1.50
4	C	801	DCA	CDP-CBP	-2.38	1.48	1.53
3	C	800	B12	C13-C14	-2.36	1.48	1.52
3	A	800	B12	C54-C17	2.32	1.58	1.54
3	A	800	B12	C6M-C6B	-2.31	1.46	1.51
3	C	800	B12	C46-C12	2.28	1.58	1.54
3	A	800	B12	C3R-C4R	2.26	1.58	1.52
3	C	800	B12	C10-C9	-2.25	1.32	1.39
3	A	800	B12	O58-C57	-2.24	1.18	1.23
3	C	800	B12	C11-N23	2.23	1.41	1.36
4	A	801	DCA	P2A-O5A	-2.22	1.45	1.55
3	A	800	B12	C11-N23	2.22	1.41	1.36
3	A	800	B12	C30-C3	2.19	1.59	1.54
3	A	800	B12	C48-C13	2.17	1.59	1.54
3	A	800	B12	C7B-C6B	2.16	1.42	1.39
4	C	801	DCA	P3B-O8A	-2.16	1.46	1.54
3	A	800	B12	C12-C11	-2.13	1.48	1.52
3	C	800	B12	P-O4	-2.10	1.43	1.50
3	C	800	B12	C7-C6	2.10	1.59	1.54
4	C	801	DCA	P1A-O3A	2.10	1.61	1.59
3	A	800	B12	O2-C3R	-2.09	1.37	1.44
3	C	800	B12	C3-C4	-2.09	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	P-O5	-2.04	1.45	1.55
3	C	800	B12	C60-C61	2.00	1.57	1.51

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C9-N22-C6	9.74	117.00	105.28
3	C	800	B12	C19-N24-C16	7.90	115.92	107.29
3	C	800	B12	C13-C14-C15	-6.92	113.80	124.32
3	A	800	B12	C13-C14-N23	6.78	118.27	109.09
5	C	802	GOL	O3-C3-C2	6.38	139.09	110.38
3	C	800	B12	C9B-C8B-N1B	6.16	108.03	105.30
3	A	800	B12	C9B-C8B-N1B	6.07	108.00	105.30
3	A	800	B12	C12-C11-C10	-5.99	115.68	123.40
3	A	800	B12	C9-N22-C6	5.85	112.32	105.28
3	A	800	B12	C13-C14-C15	-5.77	115.54	124.32
3	C	800	B12	C13-C14-N23	5.59	116.66	109.09
3	A	800	B12	C3-C4-N21	5.48	118.80	111.98
3	A	800	B12	C16-C15-C14	-5.44	112.96	121.26
3	C	800	B12	C3-C4-N21	5.42	118.72	111.98
3	C	800	B12	C12-C11-N23	5.41	119.28	111.83
3	C	800	B12	C41-C42-C43	5.41	130.93	112.55
3	C	800	B12	C2P-C1P-N59	-5.28	105.15	112.92
4	C	801	DCA	C7P-N8P-C9P	-5.17	113.26	122.55
3	A	800	B12	C12-C11-N23	4.97	118.68	111.83
3	A	800	B12	C19-N24-C16	4.96	112.71	107.29
3	A	800	B12	C55-C56-C57	-4.93	100.25	111.25
3	A	800	B12	C2P-C1P-N59	-4.83	105.81	112.92
3	C	800	B12	C10-C9-N22	4.83	131.25	125.74
3	C	800	B12	C1P-N59-C57	-4.59	112.84	122.69
3	A	800	B12	C1-C19-N24	-4.58	101.15	106.25
3	C	800	B12	C25-C2-C1	4.55	120.55	113.75
3	A	800	B12	C1P-N59-C57	-4.53	112.96	122.69
3	C	800	B12	O44-C43-N45	-4.49	110.53	122.53
3	A	800	B12	C53-C15-C14	4.47	127.28	118.42
3	A	800	B12	C25-C2-C1	4.45	120.41	113.75
3	A	800	B12	C55-C17-C18	4.41	119.54	111.12
3	C	800	B12	C30-C31-C32	4.37	127.40	112.55
3	A	800	B12	C56-C55-C17	-4.29	107.32	115.58
3	C	800	B12	C36-C7-C8	-4.13	104.43	112.05
4	A	801	DCA	CEP-CBP-CCP	4.04	114.89	108.22
3	A	800	B12	C41-C8-C9	-4.01	104.19	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C54-C17-C16	-4.00	91.69	112.41
3	C	800	B12	C2-C1-N21	3.99	107.32	101.78
3	C	800	B12	C16-C15-C14	-3.97	115.20	121.26
3	C	800	B12	O44-C43-C42	3.91	132.87	121.04
3	C	800	B12	C55-C17-C18	3.91	118.58	111.12
5	D	1	GOL	C3-C2-C1	3.88	126.01	111.80
3	C	800	B12	C49-C50-N52	3.79	128.63	116.49
3	C	800	B12	C20-C1-C19	3.78	112.99	109.35
3	C	800	B12	C1-C2-C3	-3.76	96.87	101.60
3	A	800	B12	O5-P-O4	3.75	129.87	112.44
3	C	800	B12	C2-C1-C19	-3.74	112.80	118.61
3	C	800	B12	C37-C7-C8	3.69	118.11	108.37
4	A	801	DCA	C7P-N8P-C9P	-3.62	116.04	122.55
3	C	800	B12	C7B-C8B-C9B	3.58	126.77	122.47
3	C	800	B12	C12-C11-C10	-3.53	118.85	123.40
3	C	800	B12	C54-C17-C16	-3.51	94.21	112.41
3	A	800	B12	C8B-N1B-C2B	-3.49	103.09	106.26
3	A	800	B12	C36-C7-C8	-3.38	105.80	112.05
3	A	800	B12	C9-C10-C11	-3.36	121.17	125.97
5	A	802	GOL	O3-C3-C2	3.35	125.45	110.38
3	C	800	B12	O51-C50-C49	-3.32	111.03	121.04
3	C	800	B12	O28-C27-N29	-3.29	113.75	122.53
3	A	800	B12	C5-C4-N21	-3.28	118.91	124.19
3	C	800	B12	O5-P-O4	3.24	127.51	112.44
3	C	800	B12	C56-C55-C17	-3.19	109.44	115.58
3	C	800	B12	C42-C41-C8	3.18	123.67	114.65
3	C	800	B12	C7B-C8B-N1B	-3.14	125.19	131.39
4	A	801	DCA	CDP-CBP-CAP	-3.12	103.46	108.77
4	C	801	DCA	O9P-C9P-N8P	3.05	129.43	122.98
3	A	800	B12	C37-C7-C8	3.03	116.37	108.37
3	C	800	B12	C47-C12-C11	3.03	120.90	110.08
3	A	800	B12	C2-C1-N21	3.02	105.98	101.78
3	C	800	B12	C8B-C9B-N3B	-2.92	106.84	110.00
3	A	800	B12	O51-C50-C49	-2.91	112.27	121.04
3	C	800	B12	C9-C10-C11	-2.83	121.92	125.97
3	C	800	B12	C5-C4-N21	-2.81	119.67	124.19
3	C	800	B12	C4B-C5B-C6B	2.79	123.79	119.69
3	A	800	B12	O63-C61-C60	-2.78	115.06	120.87
4	A	801	DCA	C3P-N4P-C5P	-2.77	117.92	122.57
3	A	800	B12	C4B-C5B-C6B	2.76	123.73	119.69
3	A	800	B12	N1B-C2B-N3B	2.71	117.78	113.94
3	C	800	B12	C53-C15-C16	2.68	124.91	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801	DCA	C5A-N7A-C8A	-2.67	99.25	103.45
4	C	801	DCA	O8A-P3B-O7A	2.67	121.23	110.83
3	C	800	B12	C9B-C4B-C5B	-2.67	115.89	120.83
3	C	800	B12	C8-C9-C10	-2.63	117.74	123.33
3	A	800	B12	C30-C3-C4	2.62	115.81	109.66
3	C	800	B12	C8B-C7B-C6B	-2.60	113.99	119.22
3	A	800	B12	C7B-C8B-C9B	2.59	125.58	122.47
3	A	800	B12	C2-C1-C19	-2.59	114.59	118.61
3	C	800	B12	C55-C17-C16	2.56	121.60	116.59
3	C	800	B12	C41-C8-C9	-2.55	106.74	111.19
3	A	800	B12	C26-C27-N29	2.53	124.34	116.49
3	A	800	B12	O6R-C1R-C2R	-2.53	101.21	106.62
4	C	801	DCA	C4A-C5A-N7A	2.52	113.47	110.58
3	A	800	B12	C7B-C8B-N1B	-2.52	126.41	131.39
3	C	800	B12	C8-C7-C6	2.52	105.19	100.92
3	A	800	B12	O58-C57-C56	-2.51	117.47	122.02
4	C	801	DCA	O9P-C9P-CAP	-2.43	114.12	120.89
3	A	800	B12	C48-C13-C14	2.42	114.53	108.51
3	C	800	B12	C49-C48-C13	-2.37	107.92	114.65
3	C	800	B12	C12-C13-C14	-2.35	98.39	102.26
3	C	800	B12	C55-C56-C57	-2.34	106.03	111.25
3	C	800	B12	C26-C27-N29	2.34	123.73	116.49
4	C	801	DCA	O6A-CCP-CBP	-2.33	106.80	110.55
4	C	801	DCA	C3P-N4P-C5P	-2.33	118.66	122.57
3	C	800	B12	O6R-C1R-C2R	-2.32	101.65	106.62
3	A	800	B12	C36-C7-C37	2.31	114.66	110.74
3	A	800	B12	C9B-C4B-C5B	-2.30	116.57	120.83
3	A	800	B12	C12-C13-C14	-2.28	98.51	102.26
3	A	800	B12	O28-C27-N29	-2.27	116.46	122.53
4	C	801	DCA	C1B-N9A-C8A	2.26	132.10	127.09
4	C	801	DCA	O5B-C5B-C4B	2.25	116.65	108.99
3	C	800	B12	C15-C14-N23	2.25	128.97	126.26
3	A	800	B12	C48-C13-C12	-2.23	110.15	116.52
3	A	800	B12	C42-C41-C8	-2.22	108.36	114.65
4	A	801	DCA	O8A-P3B-O7A	2.21	119.44	110.83
4	C	801	DCA	CDP-CBP-CAP	-2.15	105.10	108.77
3	C	800	B12	C31-C32-N33	2.15	123.37	116.49
4	C	801	DCA	C5A-C4A-N3A	2.14	129.66	126.72
3	C	800	B12	C54-C17-C55	-2.12	105.74	109.27
3	C	800	B12	C5M-C5B-C6B	-2.12	116.43	120.76
3	C	800	B12	C18-C60-C61	-2.11	108.68	114.04
3	A	800	B12	O2-C3R-C2R	2.10	119.22	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801	DCA	OAP-CAP-CBP	-2.10	105.31	110.18
3	A	800	B12	O3-C2P-C1P	-2.09	102.80	106.94
3	A	800	B12	O2-P-O3	-2.09	97.04	102.87
3	C	800	B12	C31-C30-C3	-2.08	108.76	114.65
3	A	800	B12	C47-C12-C11	2.06	117.45	110.08
3	C	800	B12	C35-C5-C6	2.06	125.73	122.41
3	C	800	B12	C30-C3-C2	-2.04	114.50	119.00
3	C	800	B12	C56-C57-N59	-2.02	112.65	116.34

There are no chirality outliers.

All (37) 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
5	B	639	GOL	C1-C2-C3-O3
5	B	640	GOL	C1-C2-C3-O3
5	D	1	GOL	O1-C1-C2-C3
5	D	1	GOL	C1-C2-C3-O3
3	A	800	B12	C42-C41-C8-C7
3	C	800	B12	C8-C41-C42-C43
3	A	800	B12	C16-C17-C55-C56
5	B	640	GOL	O1-C1-C2-C3
5	D	639	GOL	C1-C2-C3-O3
3	A	800	B12	C2R-C1R-N1B-C8B
3	C	800	B12	C2R-C1R-N1B-C8B
3	C	800	B12	C30-C31-C32-O34
5	B	639	GOL	O2-C2-C3-O3
5	B	640	GOL	O2-C2-C3-O3
4	C	801	DCA	P2A-O3A-P1A-O1A
3	A	800	B12	O6R-C1R-N1B-C8B
3	C	800	B12	O6R-C1R-N1B-C8B
3	C	800	B12	C30-C31-C32-N33
3	A	800	B12	C41-C42-C43-O44
3	A	800	B12	C41-C42-C43-N45
4	A	801	DCA	P2A-O3A-P1A-O2A
4	C	801	DCA	P2A-O3A-P1A-O2A
5	B	640	GOL	O1-C1-C2-O2
5	D	1	GOL	O1-C1-C2-O2
4	A	801	DCA	P2A-O3A-P1A-O1A
3	A	800	B12	C18-C60-C61-O63

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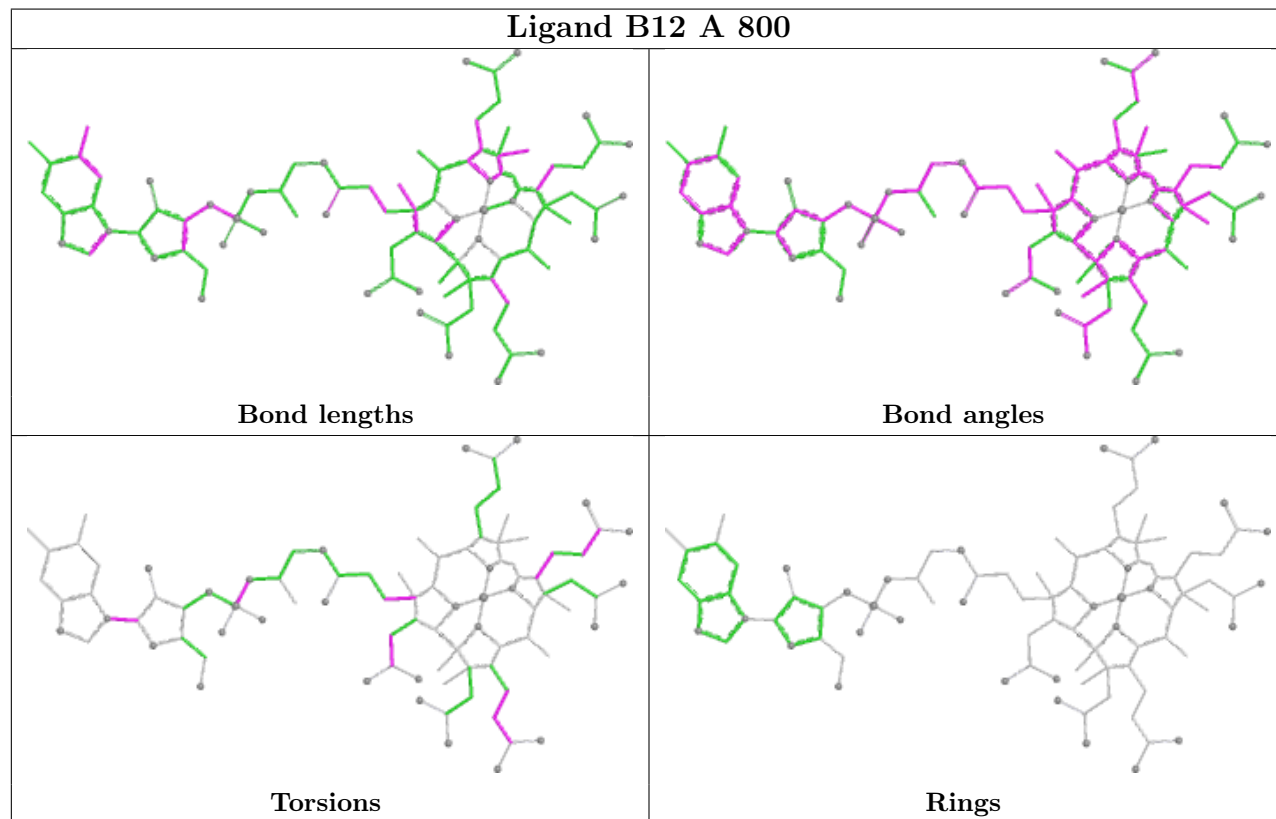
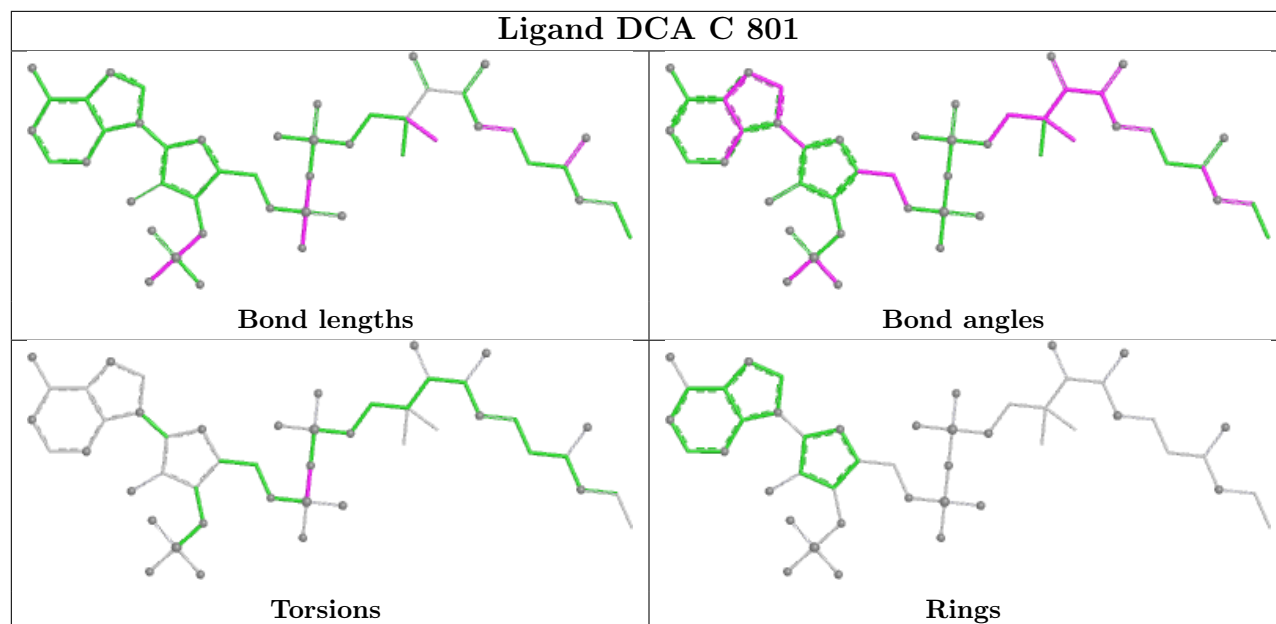
Mol	Chain	Res	Type	Atoms
3	A	800	B12	C30-C31-C32-N33
3	A	800	B12	C3-C30-C31-C32
3	A	800	B12	C2P-O3-P-O4
3	A	800	B12	C2P-O3-P-O5
3	C	800	B12	C2P-O3-P-O4
3	C	800	B12	C2P-O3-P-O5
5	D	639	GOL	O2-C2-C3-O3
3	C	800	B12	C55-C56-C57-O58

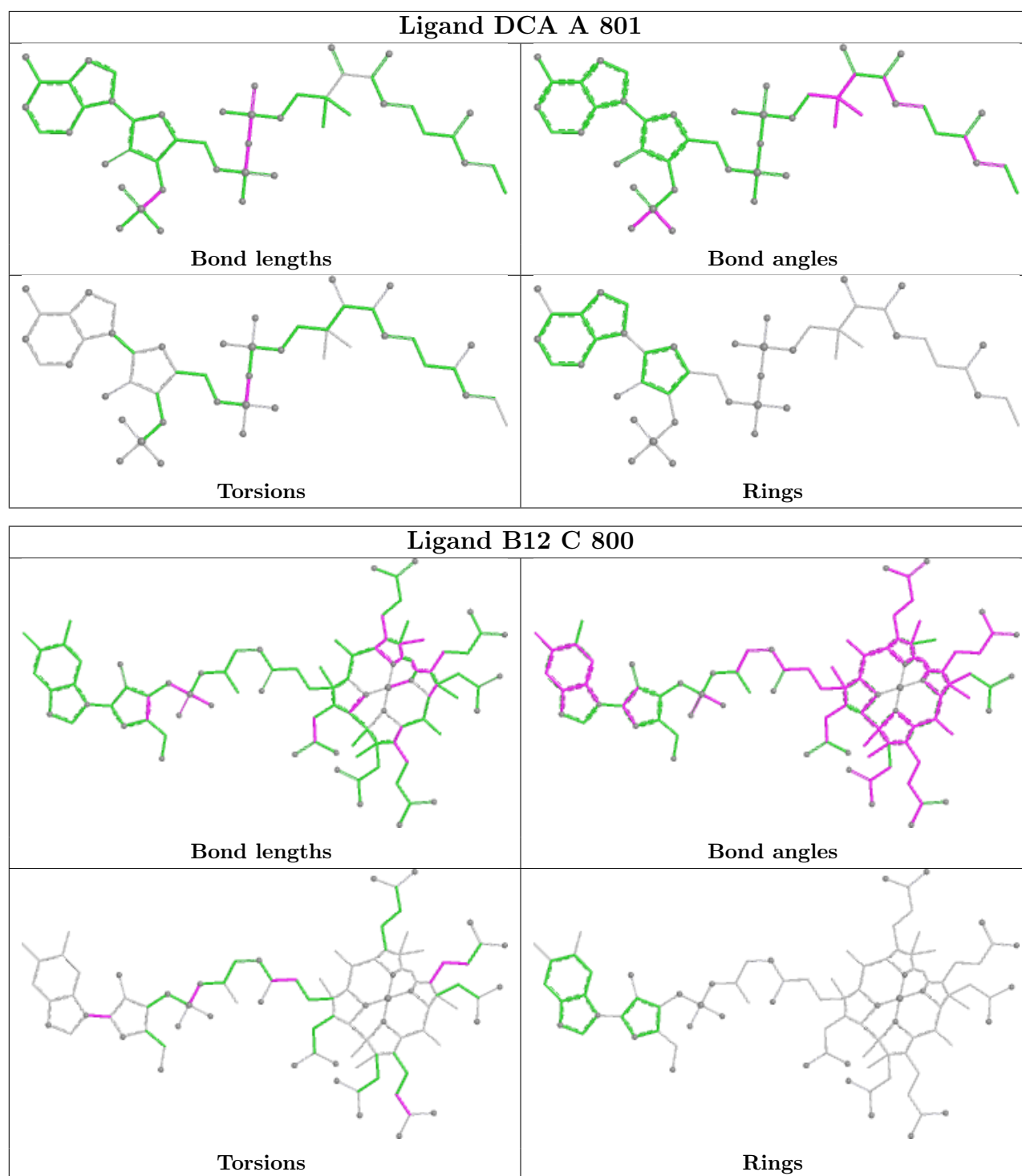
There are no ring outliers.

7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	802	GOL	3	0
5	B	640	GOL	1	0
5	C	802	GOL	3	0
5	D	1	GOL	1	0
3	A	800	B12	13	0
3	C	800	B12	10	0
5	B	639	GOL	1	0

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/727 (100%)	0.75	86 (11%) 9 8	19, 35, 61, 89	0
1	C	727/727 (100%)	0.76	79 (10%) 10 9	18, 34, 60, 105	0
2	B	619/637 (97%)	1.06	103 (16%) 4 4	23, 41, 61, 82	0
2	D	622/637 (97%)	1.83	247 (39%) 1 1	23, 50, 75, 103	0
All	All	2695/2728 (98%)	1.08	515 (19%) 3 3	18, 39, 67, 105	0

All (515) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	THR	7.4
2	D	190	ALA	6.9
1	A	3	THR	6.5
2	D	183	TYR	6.5
1	C	2	SER	5.8
2	D	273	ALA	5.5
2	D	224	LEU	5.4
2	D	199	LEU	5.3
2	D	146	ALA	5.3
2	D	191	LYS	5.2
1	A	576	ASN	5.1
1	A	5	PRO	5.1
1	A	676	GLY	4.9
2	D	91	ALA	4.9
1	C	4	LEU	4.9
1	A	477	PRO	4.9
1	C	23	ARG	4.9
2	B	432	ALA	4.8
2	D	193	LEU	4.8
2	D	225	ALA	4.8
2	D	158	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	214	LEU	4.7
1	A	481	LEU	4.6
1	C	17	VAL	4.6
2	B	146	ALA	4.6
2	D	145	ILE	4.6
2	B	190	ALA	4.5
2	D	438	VAL	4.5
2	D	233	ALA	4.5
2	B	603	GLY	4.5
2	D	189	PRO	4.5
1	C	5	PRO	4.5
2	D	87	TYR	4.4
1	C	575	LYS	4.4
2	D	432	ALA	4.4
2	D	204	PHE	4.4
2	D	423	VAL	4.4
1	C	35	GLY	4.3
2	D	262	TYR	4.3
1	C	728	ALA	4.2
1	C	574	VAL	4.2
2	D	217	LEU	4.2
2	B	265	ALA	4.2
2	D	197	LEU	4.2
1	C	10	VAL	4.2
2	D	89	GLY	4.2
2	D	159	LEU	4.2
2	D	433	VAL	4.2
2	D	307	ILE	4.1
2	D	106	ALA	4.1
2	D	195	LEU	4.1
1	A	700	GLY	4.1
2	D	194	ALA	4.1
1	C	12	LEU	4.0
2	D	420	PHE	4.0
2	D	270	GLY	4.0
2	D	313	VAL	4.0
1	A	4	LEU	4.0
2	D	234	VAL	4.0
2	D	482	ALA	3.9
1	A	488	VAL	3.9
1	C	25	PHE	3.9
2	B	183	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	308	GLY	3.9
2	B	20	THR	3.9
2	D	17	THR	3.9
2	D	187	ASP	3.9
1	C	475	GLU	3.9
2	D	182	VAL	3.9
2	D	263	VAL	3.9
1	C	15	ALA	3.9
1	A	664	LEU	3.9
2	D	441	VAL	3.8
2	D	257	ALA	3.8
2	D	276	ALA	3.8
1	A	693	PHE	3.8
2	D	173	GLY	3.8
2	D	150	LEU	3.8
1	C	13	GLY	3.8
1	C	32	ALA	3.7
2	D	229	PRO	3.7
1	A	491	GLU	3.7
2	D	221	VAL	3.7
2	D	179	LEU	3.7
2	D	151	ASP	3.7
2	D	178	ALA	3.7
2	D	136	LEU	3.6
2	D	271	PHE	3.6
1	A	473	GLU	3.6
2	D	279	THR	3.6
2	D	116	PRO	3.6
2	D	147	PRO	3.6
2	D	488	LEU	3.6
2	D	481	ALA	3.5
2	D	486	LYS	3.5
2	B	266	LEU	3.5
2	D	266	LEU	3.5
1	A	134	GLY	3.5
2	D	241	TYR	3.5
2	B	638	LYS	3.5
2	D	638	LYS	3.5
2	B	225	ALA	3.5
2	D	176	ALA	3.5
1	A	726	LEU	3.5
1	C	49	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	203	GLY	3.5
2	D	185	ARG	3.5
2	D	275	GLU	3.5
2	D	280	ILE	3.5
2	B	191	LYS	3.5
2	D	573	VAL	3.5
2	D	220	TRP	3.4
2	D	265	ALA	3.4
2	D	439	THR	3.4
1	A	2	SER	3.4
1	A	675	LEU	3.4
2	B	633	ILE	3.4
2	D	259	GLY	3.4
2	B	606	ALA	3.4
2	D	175	ALA	3.4
2	D	484	ALA	3.4
2	D	93	PHE	3.4
1	C	576	ASN	3.4
2	D	215	THR	3.4
2	D	485	ARG	3.4
1	C	480	VAL	3.4
2	D	157	VAL	3.4
2	D	201	PRO	3.4
2	D	316	ASP	3.3
1	A	480	VAL	3.3
1	A	678	PRO	3.3
2	D	310	VAL	3.3
2	D	253	ALA	3.3
2	B	189	PRO	3.3
2	B	216	VAL	3.3
2	D	180	VAL	3.3
1	A	501	ALA	3.3
2	D	300	LEU	3.3
2	D	426	LEU	3.3
2	D	277	PHE	3.3
2	B	587	ALA	3.3
2	B	598	ALA	3.3
2	D	138	LEU	3.3
1	C	572	LYS	3.3
2	D	200	ASP	3.3
1	C	14	ASN	3.2
2	D	154	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	16	PRO	3.2
2	D	78	PRO	3.2
2	D	483	PRO	3.2
2	D	188	LYS	3.2
2	D	117	ASP	3.2
2	D	227	PHE	3.2
1	A	577	THR	3.2
1	C	474	HIS	3.2
2	D	46	GLY	3.2
2	D	216	VAL	3.2
1	C	19	ALA	3.2
2	D	205	ALA	3.2
2	D	148	GLU	3.2
2	D	272	THR	3.2
1	C	21	ALA	3.1
2	D	153	VAL	3.1
2	B	436	GLU	3.1
2	D	231	SER	3.1
2	D	274	THR	3.1
1	A	508	VAL	3.1
1	A	728	ALA	3.1
2	D	67	VAL	3.1
2	D	232	ARG	3.1
2	B	634	LEU	3.1
2	D	184	GLU	3.1
2	D	431	LYS	3.1
1	A	476	PRO	3.1
1	C	18	PRO	3.1
1	A	438	GLU	3.1
2	D	267	VAL	3.1
1	A	575	LYS	3.1
1	C	407	ALA	3.1
1	C	64	TYR	3.0
1	C	34	THR	3.0
1	C	6	ARG	3.0
1	A	647	ALA	3.0
2	D	434	MET	3.0
1	A	689	PRO	3.0
1	C	7	PHE	3.0
1	C	8	ASP	3.0
2	B	144	ALA	3.0
2	B	588	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	430	VAL	3.0
2	B	423	VAL	3.0
2	D	169	ARG	3.0
2	D	202	ILE	3.0
1	C	33	GLY	3.0
2	D	77	ARG	3.0
2	D	206	ALA	3.0
2	D	198	GLY	3.0
1	C	476	PRO	3.0
2	D	82	PRO	3.0
2	D	226	LYS	3.0
2	D	282	PHE	3.0
2	D	186	SER	2.9
2	B	193	LEU	2.9
2	D	577	GLN	2.9
1	A	154	ALA	2.9
1	C	22	ALA	2.9
2	D	303	ALA	2.9
2	D	444	ALA	2.9
2	D	589	GLY	2.9
1	A	483	VAL	2.9
2	D	166	VAL	2.9
2	D	425	LYS	2.9
2	D	284	VAL	2.9
2	D	637	ALA	2.9
2	D	149	HIS	2.9
2	B	185	ARG	2.8
1	A	574	VAL	2.8
1	A	487	THR	2.8
1	A	694	ASP	2.8
2	D	410	ARG	2.8
2	B	434	MET	2.8
2	B	484	ALA	2.8
2	B	214	LEU	2.8
2	D	304	TRP	2.8
2	D	99	VAL	2.8
2	D	409	THR	2.8
1	C	11	ASP	2.8
1	C	55	TYR	2.8
1	A	662	LEU	2.8
1	A	663	THR	2.8
1	A	130	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	44	ILE	2.8
2	D	118	GLU	2.8
2	D	312	GLY	2.8
2	D	428	GLY	2.8
1	C	30	ALA	2.8
2	B	224	LEU	2.8
2	D	112	LEU	2.8
2	D	18	PRO	2.8
2	D	107	TRP	2.8
1	A	475	GLU	2.7
2	B	635	GLY	2.7
2	D	524	PHE	2.7
1	A	593	ALA	2.7
2	D	556	ALA	2.7
1	A	696	LEU	2.7
2	B	186	SER	2.7
2	D	417	TRP	2.7
1	A	513	ASP	2.7
1	C	501	ALA	2.7
1	A	478	LEU	2.7
2	B	212	PRO	2.7
2	B	148	GLU	2.7
2	B	605	ASP	2.7
1	A	517	TRP	2.7
2	B	188	LYS	2.7
2	D	126	LEU	2.7
2	D	258	THR	2.7
1	C	9	SER	2.7
1	A	727	ASP	2.7
2	B	206	ALA	2.6
2	D	590	ALA	2.6
2	D	606	ALA	2.6
2	D	480	PRO	2.6
1	A	479	ASP	2.6
2	B	170	TYR	2.6
1	A	6	ARG	2.6
1	C	274	GLY	2.6
2	D	96	GLY	2.6
2	D	422	GLU	2.6
2	D	490	TRP	2.6
1	A	701	ALA	2.6
1	A	157	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	116	PRO	2.6
2	B	593	LEU	2.6
2	B	612	LEU	2.6
2	D	120	PHE	2.6
2	D	311	PHE	2.6
2	D	479	PHE	2.6
2	B	151	ASP	2.6
2	B	591	LYS	2.6
2	D	222	ARG	2.6
1	A	230	ALA	2.6
1	A	494	ALA	2.6
1	C	439	LYS	2.6
1	C	481	LEU	2.6
2	D	53	LEU	2.6
2	D	369	LEU	2.6
1	A	430	VAL	2.6
2	D	635	GLY	2.6
1	A	139	ALA	2.6
2	D	324	ALA	2.6
2	B	49	PRO	2.6
2	D	137	LEU	2.6
1	C	438	GLU	2.5
2	D	261	GLU	2.5
1	A	670	LYS	2.5
1	C	56	LYS	2.5
2	D	105	ASP	2.5
1	C	477	PRO	2.5
1	A	671	GLU	2.5
2	D	152	GLU	2.5
2	B	145	ILE	2.5
2	D	170	TYR	2.5
1	A	485	ASN	2.5
2	D	219	ASP	2.5
2	D	435	THR	2.5
1	C	428	GLU	2.5
2	D	212	PRO	2.5
2	D	331	LEU	2.5
2	B	204	PHE	2.5
2	D	393	GLY	2.5
1	C	563	ILE	2.5
2	B	180	VAL	2.5
2	D	228	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	174	ALA	2.5
2	B	607	ALA	2.5
2	D	144	ALA	2.5
2	D	415	ALA	2.5
2	B	159	LEU	2.5
2	B	585	LEU	2.5
2	B	149	HIS	2.5
2	D	507	VAL	2.4
2	B	632	ASP	2.4
2	D	50	GLU	2.4
2	D	213	ASP	2.4
2	D	19	THR	2.4
2	D	181	SER	2.4
1	A	505	PRO	2.4
2	B	197	LEU	2.4
2	D	611	LYS	2.4
1	C	473	GLU	2.4
2	B	580	GLU	2.4
2	D	90	VAL	2.4
2	B	48	PRO	2.4
1	C	494	ALA	2.4
2	D	51	LYS	2.4
2	D	260	ALA	2.4
1	A	708	GLY	2.4
2	D	230	ASP	2.4
2	D	70	ILE	2.4
2	D	140	VAL	2.4
2	B	505	THR	2.4
2	B	586	LYS	2.4
1	A	527	PRO	2.4
1	C	45	PRO	2.4
1	C	490	ALA	2.4
2	D	130	GLU	2.4
2	D	281	ASN	2.4
2	D	604	ASP	2.4
1	A	92	PHE	2.4
2	B	310	VAL	2.4
2	D	163	LYS	2.4
1	C	510	ALA	2.3
2	D	309	GLU	2.3
1	A	489	LEU	2.3
2	B	158	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	369	LEU	2.3
2	D	21	LEU	2.3
2	D	172	GLN	2.3
2	B	487	GLY	2.3
2	D	247	GLY	2.3
1	C	20	ASP	2.3
2	B	192	ASP	2.3
2	D	192	ASP	2.3
2	D	591	LYS	2.3
1	A	585	GLU	2.3
2	B	50	GLU	2.3
2	B	147	PRO	2.3
1	A	691	GLN	2.3
1	A	724	ALA	2.3
1	C	154	ALA	2.3
2	D	489	ALA	2.3
2	D	196	ASN	2.3
1	A	586	LEU	2.3
1	C	28	LEU	2.3
2	D	612	LEU	2.3
2	D	558	LYS	2.3
2	B	155	SER	2.3
2	B	228	SER	2.3
1	A	474	HIS	2.3
1	A	497	VAL	2.3
1	C	497	VAL	2.3
2	B	182	VAL	2.3
2	D	395	VAL	2.3
2	D	134	THR	2.3
1	A	583	ALA	2.3
1	A	667	ALA	2.3
2	B	575	ALA	2.3
1	C	38	TRP	2.3
2	D	143	ASP	2.3
2	D	314	ASP	2.3
2	D	403	TYR	2.3
2	B	119	LYS	2.3
2	D	161	MET	2.3
1	A	592	GLN	2.3
1	C	48	THR	2.3
2	B	229	PRO	2.3
2	D	94	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	162	THR	2.3
1	A	524	ASP	2.3
2	B	590	ALA	2.3
2	D	255	ALA	2.3
2	D	440	LYS	2.3
2	D	603	GLY	2.3
2	D	43	LEU	2.3
2	D	585	LEU	2.3
1	C	486	SER	2.2
2	B	120	PHE	2.2
2	B	507	VAL	2.2
2	D	264	ARG	2.2
1	C	29	ALA	2.2
2	B	205	ALA	2.2
2	D	81	ALA	2.2
2	D	609	ALA	2.2
1	C	662	LEU	2.2
2	D	297	LEU	2.2
1	A	646	GLU	2.2
2	B	574	TYR	2.2
2	D	357	SER	2.2
1	A	590	PHE	2.2
1	A	372	ILE	2.2
1	A	698	LYS	2.2
1	C	487	THR	2.2
2	D	101	ASN	2.2
2	B	263	VAL	2.2
1	C	479	ASP	2.2
2	D	487	GLY	2.2
1	A	591	GLU	2.2
2	B	176	ALA	2.2
2	D	587	ALA	2.2
2	B	567	LEU	2.2
1	A	692	ASP	2.2
2	B	161	MET	2.2
2	D	125	ILE	2.2
2	B	267	VAL	2.2
2	D	352	VAL	2.2
1	C	431	GLY	2.2
2	D	305	ALA	2.2
2	D	413	ALA	2.2
2	B	488	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	439	LYS	2.2
2	B	572	LYS	2.2
2	D	323	ASN	2.2
1	C	517	TRP	2.2
2	B	117	ASP	2.2
2	B	483	PRO	2.1
2	D	97	THR	2.2
1	A	719	VAL	2.1
2	D	387	ALA	2.1
2	D	283	ARG	2.1
1	A	429	LYS	2.1
1	A	495	LYS	2.1
2	B	211	GLU	2.1
2	B	608	GLU	2.1
1	C	577	THR	2.1
2	D	49	PRO	2.1
2	D	520	THR	2.1
1	A	441	ILE	2.1
1	C	693	PHE	2.1
2	D	113	HIS	2.1
2	D	218	GLY	2.1
1	A	677	ARG	2.1
2	D	588	ALA	2.1
2	D	129	LEU	2.1
2	B	118	GLU	2.1
1	C	43	GLN	2.1
2	B	370	PRO	2.1
2	B	577	GLN	2.1
2	D	398	PRO	2.1
2	B	602	PHE	2.1
2	B	194	ALA	2.1
2	D	584	ALA	2.1
1	C	571	SER	2.1
2	D	85	LEU	2.1
2	D	207	LEU	2.1
2	D	256	LEU	2.1
2	B	422	GLU	2.1
1	C	504	ASP	2.1
1	C	524	ASP	2.1
2	D	108	ASP	2.1
1	A	697	ARG	2.1
2	D	437	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	589	GLY	2.1
1	C	507	LYS	2.1
1	C	508	VAL	2.1
2	B	482	ALA	2.1
2	D	299	ALA	2.1
2	D	320	ALA	2.1
2	D	436	GLU	2.0
2	B	172	GLN	2.0
2	D	242	HIS	2.0
1	A	578	PRO	2.0
1	C	619	THR	2.0
2	D	142	PRO	2.0
2	B	425	LYS	2.0
2	D	613	ILE	2.0
1	A	136	VAL	2.0
1	C	569	VAL	2.0
2	B	140	VAL	2.0
2	B	564	VAL	2.0
2	D	133	VAL	2.0
2	B	181	SER	2.0
2	D	135	SER	2.0
1	A	133	ALA	2.0
2	B	454	ALA	2.0
2	B	481	ALA	2.0
2	D	442	LEU	2.0
2	D	115	ASP	2.0
2	D	141	ASP	2.0
1	A	482	LYS	2.0
2	B	431	LYS	2.0
2	B	215	THR	2.0
2	D	210	THR	2.0
2	B	173	GLY	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

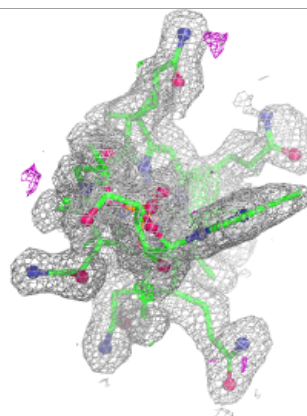
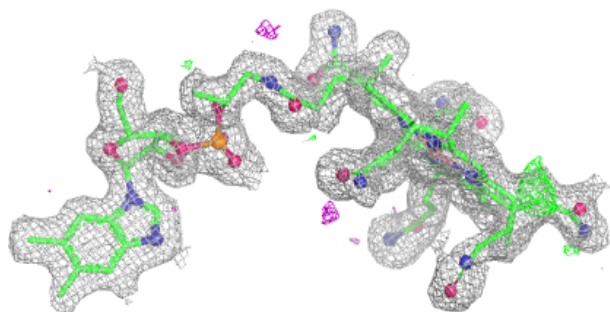
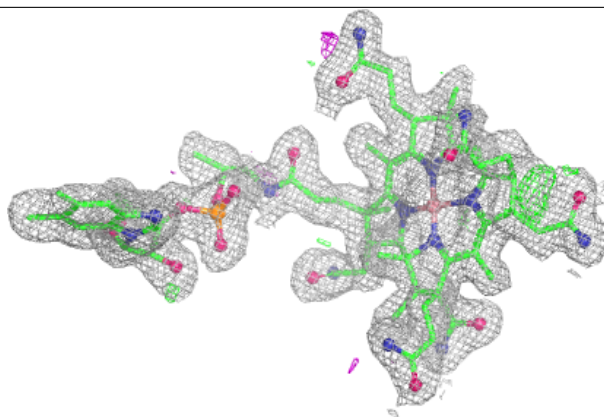
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	1	6/6	0.75	0.22	54,59,61,61	0
5	GOL	D	1	6/6	0.81	0.21	61,62,64,68	0
5	GOL	D	639	6/6	0.82	0.19	53,61,64,70	0
5	GOL	B	640	6/6	0.86	0.15	50,60,62,68	0
5	GOL	B	639	6/6	0.88	0.16	44,48,53,53	0
5	GOL	A	802	6/6	0.89	0.19	29,41,45,48	0
5	GOL	A	803	6/6	0.92	0.12	34,38,42,46	0
5	GOL	C	802	6/6	0.93	0.15	21,32,43,45	0
5	GOL	C	803	6/6	0.93	0.10	38,39,41,45	0
3	B12	A	800	91/91	0.97	0.09	17,29,48,68	0
3	B12	C	800	91/91	0.98	0.08	15,26,40,53	0
4	DCA	A	801	47/47	0.98	0.07	20,25,28,31	0
4	DCA	C	801	47/47	0.98	0.06	14,23,30,32	0

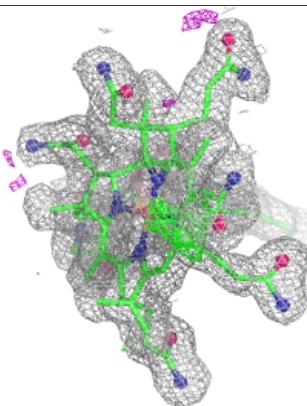
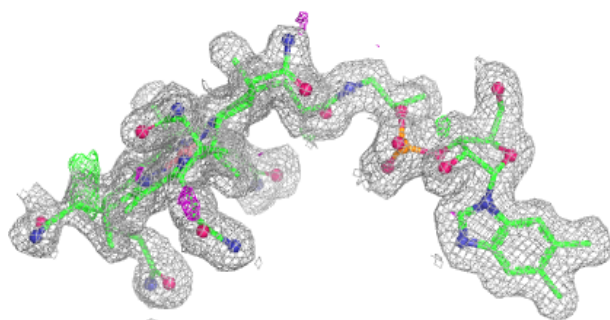
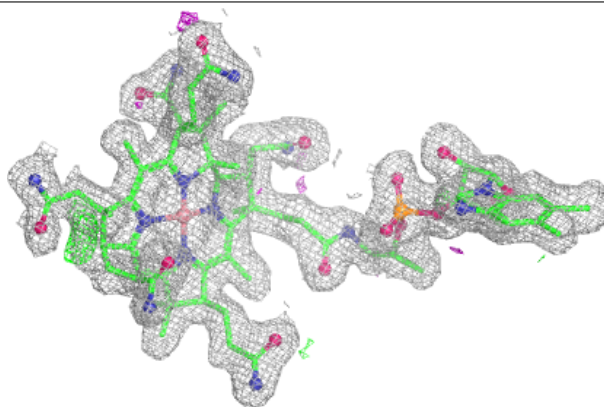
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 A 800:

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

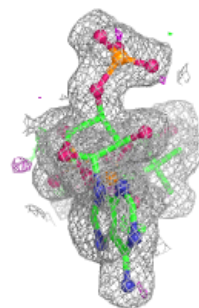
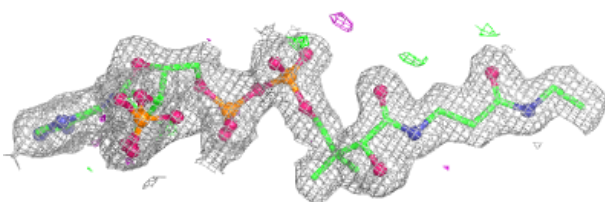
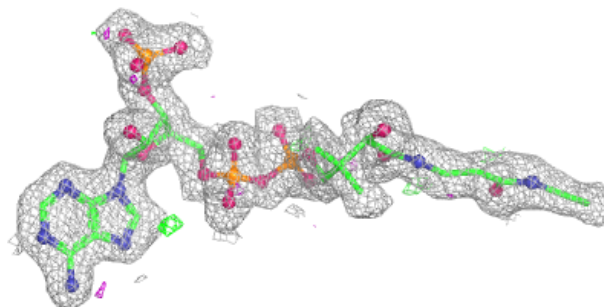
**Electron density around B12 C 800:**

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

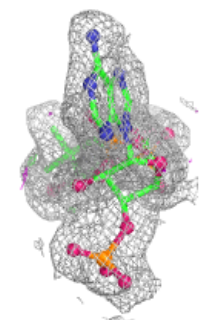
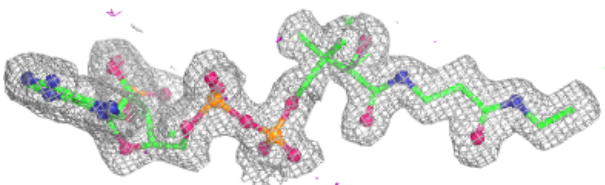
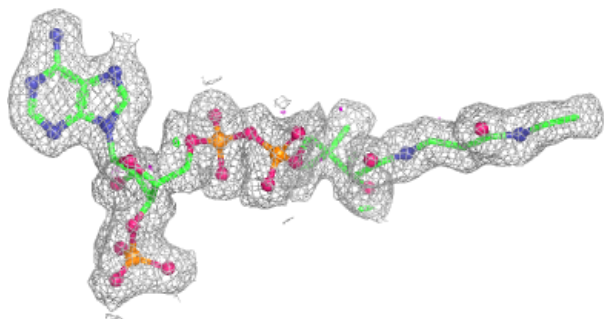


Electron density around DCA A 801:

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

**Electron density around DCA C 801:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.