



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:18 PM UTC

PDB ID : 1K0E / pdb_00001k0e
Title : THE CRYSTAL STRUCTURE OF AMINODEOXYCHORISMATE SYNTHASE FROM FORMATE GROWN CRYSTALS
Authors : Parsons, J.F.; Jensen, P.Y.; Pachikara, A.S.; Howard, A.J.; Eisenstein, E.; Ladner, J.E.
Deposited on : 2001-09-19
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
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

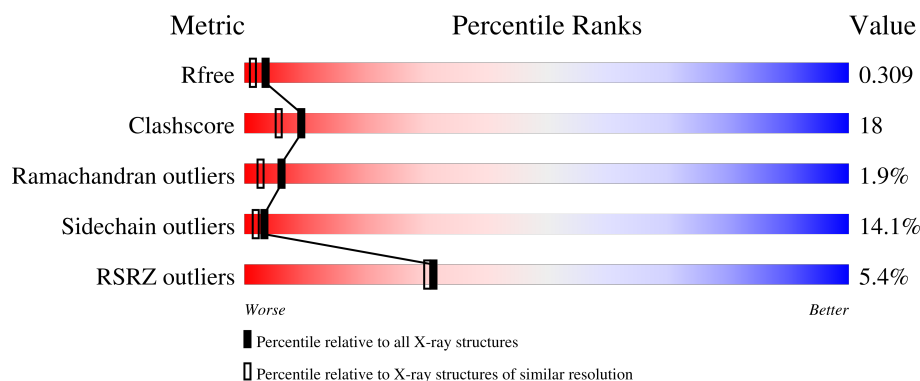
1 Overall quality at a glance

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	453	
1	B	453	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	1701	-	X	X	-

2 Entry composition [i](#)

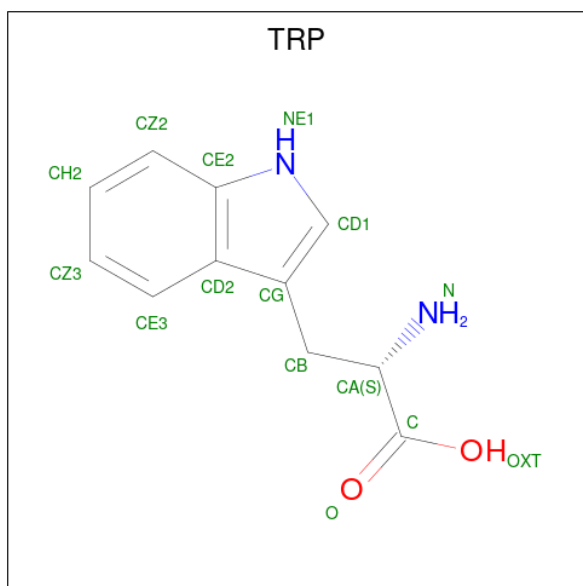
There are 4 unique types of molecules in this entry. The entry contains 7106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 p-aminobenzoate synthase component I.

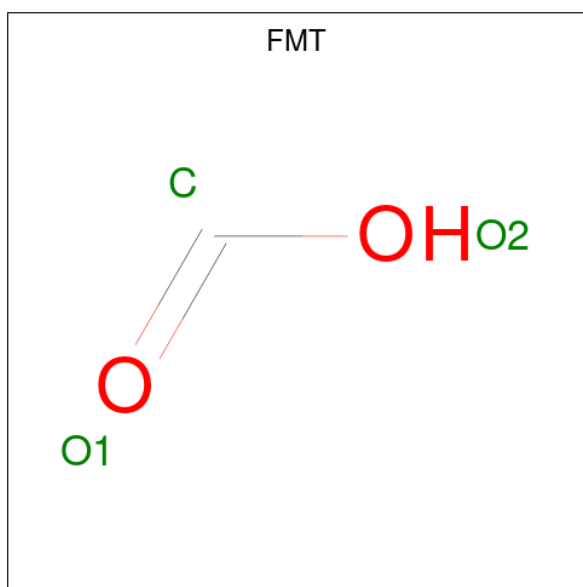
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3466	2186	605	662	13			
1	B	414	Total	C	N	O	S	0	0	0
			3289	2067	574	634	14			

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		

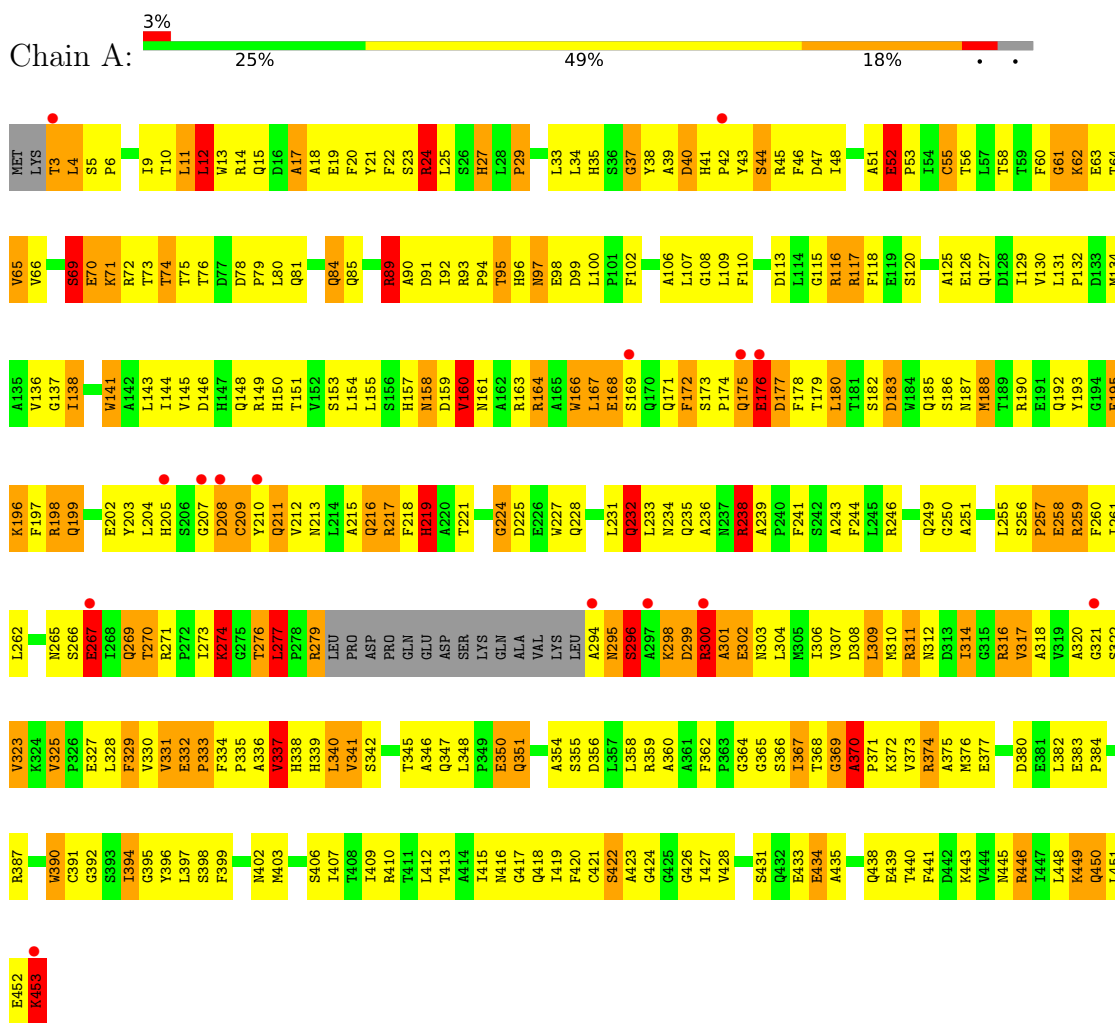
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		
4	B	132	Total	O	0	0
			132	132		

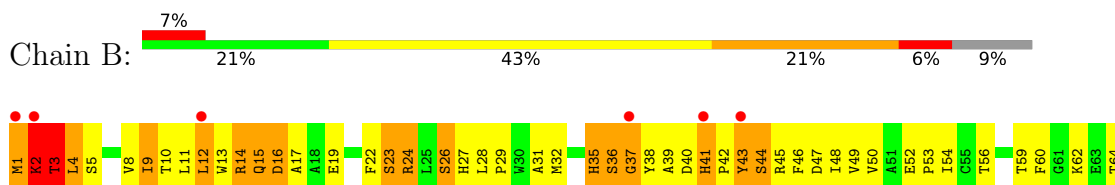
3 Residue-property plots

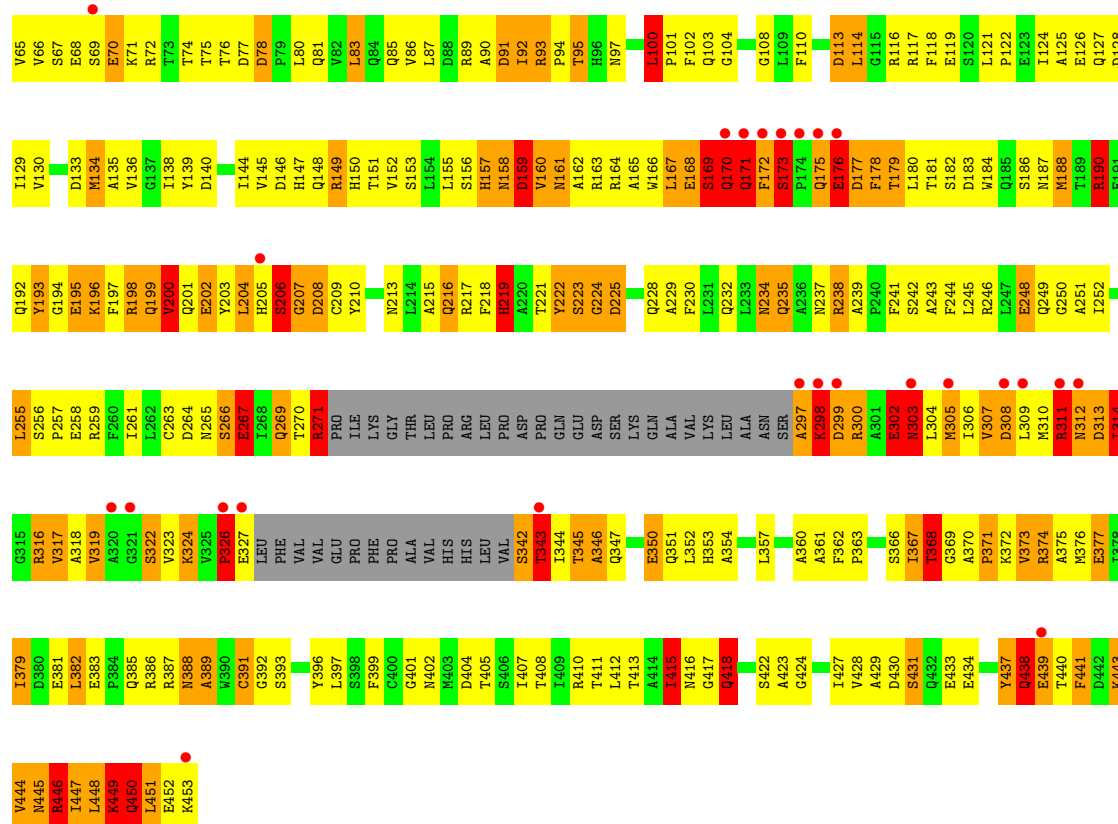
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: p-aminobenzoate synthase component I



• Molecule 1: p-aminobenzoate synthase component I





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.99Å 185.72Å 45.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.7 (10.00-2.00) 89.6 (10.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 1.84Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.205 , 0.315 0.205 , 0.309	Depositor DCC
R_{free} test set	3614 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: FMT

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	1.39	9/3543 (0.3%)	3.25	512/4813 (10.6%)
1	B	1.37	8/3357 (0.2%)	3.34	540/4552 (11.9%)
All	All	1.38	17/6900 (0.2%)	3.30	1052/9365 (11.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	GLU	C-O	15.47	1.31	1.23
1	A	157	HIS	CE1-NE2	6.70	1.39	1.32
1	A	250	GLY	C-O	6.18	1.31	1.23
1	B	144	ILE	C-O	6.04	1.30	1.24
1	A	321	GLY	N-CA	5.98	1.54	1.45
1	A	337	VAL	N-CA	-5.75	1.39	1.46
1	B	43	TYR	N-CA	-5.64	1.39	1.46
1	A	107	LEU	N-CA	5.61	1.52	1.46
1	A	21	TYR	N-CA	5.58	1.53	1.46
1	B	52	GLU	CA-CB	5.52	1.56	1.52
1	B	64	THR	N-CA	-5.24	1.39	1.46
1	B	216	GLN	C-O	5.23	1.30	1.23
1	B	200	VAL	N-CA	5.20	1.52	1.46
1	A	132	PRO	N-CD	5.12	1.54	1.47
1	A	113	ASP	N-CA	5.10	1.53	1.46
1	A	198	ARG	CD-NE	5.02	1.53	1.46
1	B	225	ASP	CA-CB	5.02	1.59	1.53

All (1052) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	GLN	CA-C-N	34.69	171.38	122.46
1	B	171	GLN	C-N-CA	34.69	171.38	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASP	CA-CB-CG	19.80	132.40	112.60
1	B	311	ARG	CD-NE-CZ	19.58	151.81	124.40
1	B	299	ASP	CA-CB-CG	17.84	130.44	112.60
1	A	316	ARG	CA-CB-CG	17.72	149.54	114.10
1	B	446	ARG	CD-NE-CZ	15.65	146.31	124.40
1	B	190	ARG	CD-NE-CZ	15.39	145.95	124.40
1	A	320	ALA	O-C-N	-15.25	102.31	122.59
1	A	172	PHE	CA-C-N	15.15	149.27	121.69
1	A	172	PHE	C-N-CA	15.15	149.27	121.69
1	B	158	ASN	CA-CB-CG	-15.14	97.46	112.60
1	A	175	GLN	CA-C-N	15.12	150.42	121.54
1	A	175	GLN	C-N-CA	15.12	150.42	121.54
1	A	174	PRO	CA-C-N	15.05	150.28	121.54
1	A	174	PRO	C-N-CA	15.05	150.28	121.54
1	B	89	ARG	CD-NE-CZ	15.04	145.45	124.40
1	A	39	ALA	O-C-N	15.03	139.89	123.06
1	B	207	GLY	CA-C-N	14.91	140.91	120.63
1	B	207	GLY	C-N-CA	14.91	140.91	120.63
1	A	89	ARG	CD-NE-CZ	14.83	145.16	124.40
1	A	311	ARG	CD-NE-CZ	14.79	145.10	124.40
1	B	415	ILE	CB-CG1-CD1	14.31	143.86	113.80
1	A	356	ASP	CA-C-O	14.09	136.02	120.10
1	A	369	GLY	O-C-N	-14.04	104.45	122.70
1	B	351	GLN	OE1-CD-NE2	-13.29	109.31	122.60
1	A	320	ALA	CA-C-N	-13.21	95.53	121.41
1	A	320	ALA	C-N-CA	-13.21	95.53	121.41
1	B	205	HIS	CA-C-N	13.12	146.60	121.54
1	B	205	HIS	C-N-CA	13.12	146.60	121.54
1	B	171	GLN	CA-C-O	-13.04	106.73	120.55
1	B	89	ARG	NE-CZ-NH2	-12.83	107.65	119.20
1	A	17	ALA	O-C-N	12.33	136.65	122.22
1	A	207	GLY	N-CA-C	12.23	131.55	115.40
1	A	295	ASN	O-C-N	12.04	136.81	122.24
1	A	356	ASP	CA-CB-CG	-12.02	100.58	112.60
1	B	418	GLN	OE1-CD-NE2	12.00	134.60	122.60
1	A	12	LEU	O-C-N	-11.91	108.77	123.06
1	A	218	PHE	CA-C-O	11.86	133.97	120.80
1	B	206	SER	CA-C-O	11.79	137.37	120.51
1	A	267	GLU	CB-CG-CD	11.77	132.61	112.60
1	B	127	GLN	OE1-CD-NE2	11.69	134.29	122.60
1	A	410	ARG	NE-CZ-NH1	11.41	132.91	121.50
1	B	163	ARG	NE-CZ-NH2	11.36	129.42	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	GLN	CA-C-O	-11.21	108.44	121.11
1	A	15	GLN	CB-CG-CD	11.14	131.54	112.60
1	A	271	ARG	CD-NE-CZ	11.13	139.99	124.40
1	A	157	HIS	N-CA-C	-11.07	99.50	113.23
1	A	159	ASP	CA-C-O	11.04	132.27	120.46
1	A	417	GLY	CA-C-N	-10.98	105.57	122.81
1	A	417	GLY	C-N-CA	-10.98	105.57	122.81
1	A	316	ARG	NH1-CZ-NH2	10.94	133.52	119.30
1	A	13	TRP	O-C-N	-10.87	109.62	122.89
1	B	257	PRO	CA-C-N	-10.87	107.17	122.93
1	B	257	PRO	C-N-CA	-10.87	107.17	122.93
1	A	266	SER	CA-C-N	-10.86	108.33	122.77
1	A	266	SER	C-N-CA	-10.86	108.33	122.77
1	B	176	GLU	CA-C-N	-10.85	106.48	122.65
1	B	176	GLU	C-N-CA	-10.85	106.48	122.65
1	A	452	GLU	CA-C-N	10.72	141.00	121.70
1	A	452	GLU	C-N-CA	10.72	141.00	121.70
1	B	219	HIS	CA-CB-CG	-10.70	103.10	113.80
1	A	316	ARG	NE-CZ-NH2	-10.65	109.61	119.20
1	A	234	ASN	CA-CB-CG	-10.58	102.02	112.60
1	A	145	VAL	CA-C-O	-10.58	108.28	120.66
1	A	146	ASP	CA-CB-CG	10.57	123.17	112.60
1	B	163	ARG	NE-CZ-NH1	-10.52	110.98	121.50
1	A	300	ARG	CD-NE-CZ	10.48	139.08	124.40
1	B	207	GLY	O-C-N	10.48	136.33	122.70
1	B	438	GLN	CA-C-O	10.46	132.13	119.79
1	A	231	LEU	CA-C-O	-10.44	109.36	120.63
1	B	89	ARG	NE-CZ-NH1	10.43	131.93	121.50
1	A	394	ILE	O-C-N	-10.26	112.10	123.18
1	A	102	PHE	CA-C-O	-10.18	109.12	120.32
1	B	270	THR	CA-C-N	10.16	140.00	121.70
1	B	270	THR	C-N-CA	10.16	140.00	121.70
1	A	80	LEU	CA-C-O	-10.15	107.82	119.79
1	B	399	PHE	CA-CB-CG	10.13	123.93	113.80
1	B	312	ASN	O-C-N	10.11	134.70	122.27
1	B	373	VAL	O-C-N	10.07	131.64	121.87
1	B	173	SER	O-C-N	-10.06	109.75	121.32
1	B	53	PRO	O-C-N	10.05	135.42	123.06
1	B	22	PHE	CA-CB-CG	-10.04	103.76	113.80
1	A	126	GLU	CA-C-O	10.04	132.40	121.16
1	A	209	CYS	CA-C-N	-10.03	106.49	122.23
1	A	209	CYS	C-N-CA	-10.03	106.49	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	CYS	CA-C-O	-9.96	110.02	121.58
1	B	352	LEU	CA-C-O	-9.94	110.26	121.89
1	A	197	PHE	O-C-N	-9.91	111.86	122.07
1	A	232	GLN	CA-CB-CG	9.85	133.80	114.10
1	B	316	ARG	CA-C-O	9.84	131.49	119.38
1	A	81	GLN	CA-C-O	9.79	130.93	120.55
1	B	323	VAL	O-C-N	9.79	133.35	122.68
1	A	12	LEU	N-CA-C	9.75	124.57	110.24
1	A	228	GLN	CA-C-O	9.72	130.85	120.55
1	A	295	ASN	CA-CB-CG	-9.72	102.88	112.60
1	A	11	LEU	CA-C-N	-9.71	107.16	121.05
1	A	11	LEU	C-N-CA	-9.71	107.16	121.05
1	A	316	ARG	CD-NE-CZ	-9.69	110.83	124.40
1	A	46	PHE	O-C-N	9.61	135.64	123.15
1	B	69	SER	CA-C-N	-9.61	106.03	122.56
1	B	69	SER	C-N-CA	-9.61	106.03	122.56
1	A	51	ALA	CA-C-O	-9.61	110.50	121.26
1	A	225	ASP	CA-CB-CG	-9.54	103.06	112.60
1	B	68	GLU	CA-C-N	-9.53	104.89	121.66
1	B	68	GLU	C-N-CA	-9.53	104.89	121.66
1	B	208	ASP	CA-C-O	9.51	130.70	120.90
1	A	427	ILE	CA-C-O	-9.49	110.42	120.39
1	A	330	VAL	CA-C-N	-9.49	107.37	122.64
1	A	330	VAL	C-N-CA	-9.49	107.37	122.64
1	B	368	THR	CA-CB-OG1	-9.48	95.37	109.60
1	B	130	VAL	O-C-N	-9.45	111.87	122.36
1	B	27	HIS	CA-CB-CG	-9.43	104.37	113.80
1	B	151	THR	CA-C-O	-9.39	109.86	120.66
1	A	69	SER	CA-C-O	9.34	133.86	120.51
1	B	242	SER	O-C-N	9.31	134.10	122.65
1	A	234	ASN	O-C-N	-9.30	112.49	122.07
1	B	139	TYR	CA-C-O	-9.30	110.66	120.70
1	B	235	GLN	CA-C-O	-9.29	109.28	119.97
1	A	150	HIS	CA-CB-CG	-9.29	104.51	113.80
1	B	95	THR	O-C-N	-9.21	111.65	122.89
1	B	164	ARG	CD-NE-CZ	9.20	137.28	124.40
1	A	359	ARG	CD-NE-CZ	9.17	137.24	124.40
1	B	43	TYR	CA-C-O	9.15	130.12	120.42
1	B	113	ASP	CA-CB-CG	-9.15	103.45	112.60
1	B	241	PHE	CA-CB-CG	-9.12	104.69	113.80
1	B	172	PHE	N-CA-C	9.11	123.69	111.30
1	B	78	ASP	O-C-N	-9.09	114.38	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	GLN	CB-CG-CD	-9.09	97.15	112.60
1	A	182	SER	O-C-N	-9.09	113.72	123.26
1	A	300	ARG	O-C-N	9.09	134.07	122.71
1	A	175	GLN	O-C-N	9.08	134.67	122.59
1	A	78	ASP	CA-CB-CG	-9.07	103.53	112.60
1	A	234	ASN	CA-C-N	9.07	132.23	120.44
1	A	234	ASN	C-N-CA	9.07	132.23	120.44
1	B	450	GLN	O-C-N	-9.07	110.53	122.59
1	B	85	GLN	CA-C-N	9.04	132.13	120.56
1	B	85	GLN	C-N-CA	9.04	132.13	120.56
1	A	160	VAL	CA-C-O	-9.02	107.72	119.53
1	B	346	ALA	CA-C-N	-8.98	107.73	122.82
1	B	346	ALA	C-N-CA	-8.98	107.73	122.82
1	A	434	GLU	CB-CG-CD	8.96	127.82	112.60
1	A	14	ARG	NH1-CZ-NH2	8.94	130.93	119.30
1	B	216	GLN	CA-C-O	-8.93	111.07	121.16
1	A	336	ALA	N-CA-C	8.92	123.46	112.23
1	B	415	ILE	CA-C-O	8.91	129.05	120.31
1	A	370	ALA	CA-C-O	8.91	132.37	120.16
1	A	339	HIS	CB-CG-CD2	8.91	142.78	131.20
1	B	67	SER	CA-C-O	-8.91	109.33	120.20
1	B	353	HIS	CA-CB-CG	-8.88	104.92	113.80
1	B	117	ARG	NE-CZ-NH2	-8.88	111.21	119.20
1	B	269	GLN	CB-CG-CD	-8.85	97.55	112.60
1	A	216	GLN	CA-C-O	-8.80	110.91	121.56
1	A	276	THR	CA-CB-CG2	8.78	125.42	110.50
1	A	108	GLY	N-CA-C	8.78	121.86	110.45
1	A	97	ASN	CA-C-O	-8.77	108.14	120.15
1	A	118	PHE	CA-C-N	8.69	136.63	122.29
1	A	118	PHE	C-N-CA	8.69	136.63	122.29
1	B	108	GLY	CA-C-O	-8.69	114.91	120.91
1	B	179	THR	CA-C-O	8.69	130.69	120.43
1	B	317	VAL	N-CA-CB	-8.69	100.39	112.12
1	A	13	TRP	CA-C-O	8.69	130.89	121.16
1	A	116	ARG	NE-CZ-NH2	8.68	127.01	119.20
1	B	196	LYS	O-C-N	8.68	131.00	122.07
1	B	36	SER	CA-C-O	8.67	130.26	119.59
1	B	194	GLY	O-C-N	-8.66	113.87	122.19
1	A	327	GLU	O-C-N	8.66	133.54	123.41
1	B	431	SER	CA-C-O	-8.66	112.12	121.99
1	A	301	ALA	CA-C-N	-8.65	108.01	120.29
1	A	301	ALA	C-N-CA	-8.65	108.01	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ARG	NE-CZ-NH2	8.65	126.98	119.20
1	A	360	ALA	CA-C-O	8.62	129.89	119.97
1	B	430	ASP	CA-CB-CG	-8.61	103.99	112.60
1	A	228	GLN	O-C-N	-8.61	112.99	122.12
1	B	300	ARG	N-CA-C	-8.60	101.84	111.82
1	B	363	PRO	CA-C-N	8.60	138.27	121.41
1	B	363	PRO	C-N-CA	8.60	138.27	121.41
1	A	413	THR	CA-C-N	8.59	135.30	123.11
1	A	413	THR	C-N-CA	8.59	135.30	123.11
1	B	177	ASP	O-C-N	8.56	133.21	123.19
1	B	36	SER	O-C-N	-8.53	111.45	122.37
1	A	219	HIS	ND1-CE1-NE2	8.53	116.93	108.40
1	A	336	ALA	CA-C-O	8.53	129.85	119.79
1	B	258	GLU	N-CA-C	8.53	123.32	109.59
1	B	307	VAL	CA-C-O	8.52	129.81	120.95
1	B	388	ASN	CA-CB-CG	-8.52	104.08	112.60
1	B	362	PHE	CA-C-O	-8.51	111.55	120.23
1	B	127	GLN	O-C-N	8.51	132.16	122.55
1	B	144	ILE	CA-C-O	-8.50	111.47	120.48
1	A	12	LEU	N-CA-CB	-8.48	96.33	109.48
1	B	213	ASN	O-C-N	-8.48	111.79	122.82
1	A	188	MET	CA-C-N	-8.47	105.40	121.66
1	A	188	MET	C-N-CA	-8.47	105.40	121.66
1	A	300	ARG	CA-C-N	8.45	137.69	121.54
1	A	300	ARG	C-N-CA	8.45	137.69	121.54
1	B	445	ASN	CA-C-O	-8.45	111.94	120.82
1	A	61	GLY	CA-C-O	8.45	132.66	121.51
1	B	161	ASN	OD1-CG-ND2	8.44	131.04	122.60
1	A	115	GLY	CA-C-O	8.41	129.02	120.45
1	A	407	ILE	N-CA-CB	8.41	122.05	111.46
1	A	374	ARG	N-CA-C	-8.40	102.08	111.82
1	A	364	GLY	CA-C-N	-8.38	109.57	120.22
1	A	364	GLY	C-N-CA	-8.38	109.57	120.22
1	A	262	LEU	O-C-N	-8.38	113.44	123.16
1	A	295	ASN	OD1-CG-ND2	8.36	130.96	122.60
1	A	34	LEU	CA-C-O	8.34	129.50	120.32
1	B	127	GLN	CA-C-O	-8.33	112.72	122.13
1	B	176	GLU	O-C-N	-8.33	112.69	122.93
1	B	438	GLN	O-C-N	-8.33	111.17	122.33
1	B	342	SER	CA-CB-OG	8.32	127.74	111.10
1	B	95	THR	N-CA-CB	-8.32	97.75	109.97
1	A	235	GLN	O-C-N	-8.31	113.51	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	GLU	O-C-N	-8.29	111.99	122.43
1	A	426	GLY	CA-C-N	-8.27	112.31	123.14
1	A	426	GLY	C-N-CA	-8.27	112.31	123.14
1	A	14	ARG	NE-CZ-NH1	-8.24	113.25	121.50
1	B	46	PHE	N-CA-C	8.24	123.06	109.95
1	A	182	SER	CA-C-O	8.24	130.11	121.38
1	B	124	ILE	CA-C-O	-8.21	110.81	120.83
1	A	374	ARG	CD-NE-CZ	-8.21	112.91	124.40
1	A	85	GLN	OE1-CD-NE2	-8.19	114.41	122.60
1	A	346	ALA	CA-C-O	-8.19	112.42	120.94
1	B	382	LEU	N-CA-CB	-8.19	99.28	110.67
1	B	452	GLU	CA-CB-CG	8.19	130.47	114.10
1	A	120	SER	O-C-N	-8.17	112.97	123.02
1	A	127	GLN	CA-C-O	-8.16	112.98	122.37
1	A	186	SER	CA-C-O	-8.16	112.18	121.81
1	A	172	PHE	O-C-N	8.15	133.03	122.43
1	A	179	THR	O-C-N	8.15	133.19	123.33
1	B	85	GLN	O-C-N	-8.12	113.51	122.12
1	B	392	GLY	N-CA-C	-8.12	101.25	112.13
1	B	41	HIS	N-CA-C	8.12	115.43	108.13
1	B	165	ALA	O-C-N	8.10	130.41	122.07
1	B	52	GLU	CA-C-O	8.10	126.71	120.48
1	B	440	THR	N-CA-C	-8.08	102.43	111.07
1	B	246	ARG	O-C-N	8.06	132.64	123.05
1	B	299	ASP	CA-C-N	-8.06	108.06	120.31
1	B	299	ASP	C-N-CA	-8.06	108.06	120.31
1	B	360	ALA	CA-C-O	8.05	129.23	119.49
1	A	146	ASP	CA-C-O	-8.05	112.14	120.84
1	A	418	GLN	N-CA-CB	-8.04	97.33	111.08
1	B	314	ILE	CA-C-O	8.04	129.18	120.57
1	A	5	SER	CA-C-N	-8.03	112.44	120.31
1	A	5	SER	C-N-CA	-8.03	112.44	120.31
1	B	119	GLU	O-C-N	8.03	134.34	123.34
1	B	145	VAL	CA-C-O	-8.03	111.94	120.53
1	B	3	THR	O-C-N	-8.03	111.81	122.97
1	B	302	GLU	CA-C-O	8.02	131.98	120.51
1	B	271	ARG	CD-NE-CZ	7.99	135.58	124.40
1	A	92	ILE	CA-C-N	-7.97	113.39	122.00
1	A	92	ILE	C-N-CA	-7.97	113.39	122.00
1	B	39	ALA	O-C-N	-7.96	113.72	123.04
1	A	342	SER	CA-CB-OG	-7.96	95.19	111.10
1	A	40	ASP	N-CA-CB	7.95	122.20	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	GLU	O-C-N	-7.94	113.79	121.18
1	B	225	ASP	N-CA-C	7.91	120.94	108.67
1	A	355	SER	CA-C-O	-7.90	111.17	120.10
1	B	64	THR	CA-C-O	-7.90	111.77	120.38
1	A	210	TYR	CA-CB-CG	7.88	128.07	113.90
1	A	116	ARG	CD-NE-CZ	-7.87	113.39	124.40
1	B	411	THR	O-C-N	-7.87	114.11	123.31
1	B	90	ALA	O-C-N	7.87	131.42	122.22
1	A	10	THR	O-C-N	-7.86	114.04	123.16
1	A	72	ARG	CA-C-O	-7.86	111.91	120.24
1	A	173	SER	O-C-N	7.85	127.59	121.47
1	B	235	GLN	N-CA-C	-7.85	102.71	111.82
1	A	241	PHE	CA-CB-CG	-7.85	105.95	113.80
1	A	219	HIS	CE1-NE2-CD2	-7.83	101.17	109.00
1	A	409	ILE	CA-C-O	-7.82	111.00	120.78
1	B	373	VAL	CA-C-O	-7.82	112.82	120.95
1	A	328	LEU	CA-C-O	7.82	129.65	120.66
1	B	140	ASP	O-C-N	7.80	131.85	122.26
1	A	150	HIS	CA-C-N	-7.78	109.45	122.29
1	A	150	HIS	C-N-CA	-7.78	109.45	122.29
1	A	203	TYR	O-C-N	-7.76	113.14	122.22
1	B	437	TYR	O-C-N	-7.76	113.89	122.12
1	B	95	THR	CB-CA-C	7.76	122.92	109.65
1	B	351	GLN	CB-CG-CD	7.76	125.79	112.60
1	A	274	LYS	CA-C-O	-7.75	109.53	120.15
1	A	334	PHE	O-C-N	7.75	127.59	121.55
1	A	339	HIS	CG-CD2-NE2	7.74	114.94	107.20
1	A	44	SER	N-CA-CB	-7.73	100.33	111.54
1	A	419	ILE	O-C-N	-7.72	114.84	123.18
1	A	246	ARG	NE-CZ-NH1	-7.72	113.78	121.50
1	A	302	GLU	CA-C-O	7.72	128.60	120.42
1	B	67	SER	O-C-N	7.72	133.16	123.28
1	A	331	VAL	CA-C-O	7.71	131.27	121.48
1	B	70	GLU	N-CA-CB	-7.69	99.32	110.47
1	B	244	PHE	CA-C-O	-7.68	112.10	120.24
1	B	56	THR	CA-C-O	7.67	129.95	121.06
1	B	42	PRO	CA-C-N	7.66	131.17	120.29
1	B	42	PRO	C-N-CA	7.66	131.17	120.29
1	A	24	ARG	CB-CA-C	-7.66	96.22	110.01
1	B	177	ASP	CA-C-O	-7.66	112.30	120.80
1	A	276	THR	CA-CB-OG1	-7.66	98.12	109.60
1	B	86	VAL	N-CA-C	-7.65	103.34	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ILE	CA-C-O	7.65	128.72	120.53
1	B	150	HIS	O-C-N	7.64	131.75	122.58
1	A	199	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	A	380	ASP	O-C-N	7.59	131.61	122.27
1	B	100	LEU	CA-C-N	7.59	127.23	119.19
1	B	100	LEU	C-N-CA	7.59	127.23	119.19
1	B	158	ASN	OD1-CG-ND2	7.59	130.19	122.60
1	A	431	SER	CA-C-O	-7.58	113.30	121.56
1	A	410	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	A	406	SER	CA-C-O	-7.57	112.04	121.88
1	A	316	ARG	CA-C-N	-7.57	108.35	121.97
1	A	316	ARG	C-N-CA	-7.57	108.35	121.97
1	B	448	LEU	O-C-N	7.54	130.12	122.12
1	A	413	THR	CA-C-O	-7.53	112.49	120.40
1	A	180	LEU	CA-C-O	-7.53	112.15	120.81
1	B	305	MET	CA-C-O	-7.52	112.44	120.42
1	A	177	ASP	CA-CB-CG	-7.52	105.08	112.60
1	B	146	ASP	CA-C-O	-7.52	112.13	120.70
1	B	230	PHE	O-C-N	-7.52	114.15	122.12
1	A	79	PRO	O-C-N	-7.49	112.56	122.22
1	A	269	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	A	221	THR	CA-C-O	-7.48	112.38	121.36
1	A	329	PHE	N-CA-CB	-7.48	97.85	110.49
1	A	392	GLY	N-CA-C	-7.46	101.81	112.55
1	B	218	PHE	CA-C-N	-7.45	109.99	122.29
1	B	218	PHE	C-N-CA	-7.45	109.99	122.29
1	B	8	VAL	CA-CB-CG2	7.45	123.06	110.40
1	B	17	ALA	N-CA-C	7.44	121.27	111.75
1	B	152	VAL	O-C-N	-7.43	113.14	122.88
1	A	328	LEU	O-C-N	-7.43	114.21	123.27
1	B	198	ARG	CA-C-N	-7.43	109.02	120.31
1	B	198	ARG	C-N-CA	-7.43	109.02	120.31
1	B	130	VAL	CA-C-O	7.42	129.57	121.70
1	A	362	PHE	N-CA-C	7.42	119.13	109.93
1	A	233	LEU	CA-C-O	7.41	128.40	120.55
1	A	426	GLY	CA-C-O	7.41	128.45	121.64
1	B	160	VAL	CA-C-N	-7.41	110.81	120.44
1	B	160	VAL	C-N-CA	-7.41	110.81	120.44
1	B	128	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	438	GLN	CA-C-N	-7.40	109.06	120.31
1	A	438	GLN	C-N-CA	-7.40	109.06	120.31
1	B	443	LYS	CA-C-N	-7.40	108.65	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	LYS	C-N-CA	-7.40	108.65	121.97
1	B	264	ASP	CA-C-O	-7.39	112.86	120.84
1	B	41	HIS	CB-CA-C	-7.39	99.90	110.03
1	B	408	THR	CA-C-O	7.39	132.17	122.63
1	A	34	LEU	O-C-N	-7.39	114.55	123.27
1	B	134	MET	CA-C-N	7.39	134.61	123.23
1	B	134	MET	C-N-CA	7.39	134.61	123.23
1	B	199	GLN	CA-C-N	-7.39	108.73	120.55
1	B	199	GLN	C-N-CA	-7.39	108.73	120.55
1	A	64	THR	CA-C-O	-7.35	112.42	120.36
1	A	337	VAL	N-CA-CB	-7.35	99.10	111.23
1	A	209	CYS	N-CA-C	7.34	120.56	109.41
1	B	87	LEU	CA-C-O	7.34	128.53	120.82
1	A	384	PRO	O-C-N	-7.33	112.42	122.24
1	A	198	ARG	CD-NE-CZ	-7.33	114.14	124.40
1	B	238	ARG	CD-NE-CZ	7.32	134.64	124.40
1	B	150	HIS	CA-C-N	-7.31	110.89	122.73
1	B	150	HIS	C-N-CA	-7.31	110.89	122.73
1	B	184	TRP	CB-CG-CD1	7.30	137.86	126.90
1	B	360	ALA	O-C-N	-7.30	112.90	122.39
1	B	206	SER	CA-C-N	7.27	135.65	121.41
1	B	206	SER	C-N-CA	7.27	135.65	121.41
1	B	12	LEU	N-CA-CB	-7.26	98.57	109.69
1	B	423	ALA	CA-C-N	-7.26	112.73	122.03
1	B	423	ALA	C-N-CA	-7.26	112.73	122.03
1	B	385	GLN	CA-C-O	-7.26	112.97	121.46
1	A	320	ALA	CA-C-O	7.25	130.88	120.51
1	A	334	PHE	CA-CB-CG	-7.25	106.55	113.80
1	B	360	ALA	CA-C-N	-7.25	110.73	122.26
1	B	360	ALA	C-N-CA	-7.25	110.73	122.26
1	B	235	GLN	CB-CG-CD	7.25	124.92	112.60
1	B	116	ARG	NE-CZ-NH1	-7.24	114.26	121.50
1	B	373	VAL	CA-C-N	-7.22	110.61	120.28
1	B	373	VAL	C-N-CA	-7.22	110.61	120.28
1	A	410	ARG	CG-CD-NE	-7.21	96.14	112.00
1	A	398	SER	CA-C-N	7.20	130.65	120.28
1	A	398	SER	C-N-CA	7.20	130.65	120.28
1	B	40	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	367	ILE	CA-C-O	7.20	126.52	119.97
1	B	190	ARG	NE-CZ-NH2	7.19	125.67	119.20
1	B	52	GLU	CB-CA-C	-7.18	104.75	111.00
1	A	18	ALA	N-CA-CB	7.17	120.38	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ARG	O-C-N	7.16	131.40	123.52
1	B	385	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	B	16	ASP	N-CA-CB	-7.16	99.60	110.91
1	B	266	SER	CA-C-N	-7.15	113.54	122.84
1	B	266	SER	C-N-CA	-7.15	113.54	122.84
1	B	234	ASN	CA-CB-CG	7.12	119.72	112.60
1	B	263	CYS	CA-C-O	7.11	128.10	120.63
1	A	125	ALA	O-C-N	-7.11	115.15	123.11
1	B	416	ASN	CA-C-N	-7.11	112.08	122.46
1	B	416	ASN	C-N-CA	-7.11	112.08	122.46
1	A	100	LEU	O-C-N	-7.11	114.98	121.37
1	A	250	GLY	CA-C-N	-7.11	111.53	122.62
1	A	250	GLY	C-N-CA	-7.11	111.53	122.62
1	B	210	TYR	CA-CB-CG	-7.11	101.11	113.90
1	B	303	ASN	CA-C-O	-7.11	112.89	120.42
1	B	40	ASP	CA-C-N	7.10	133.78	122.56
1	B	40	ASP	C-N-CA	7.10	133.78	122.56
1	B	90	ALA	CA-C-N	-7.10	112.18	122.19
1	B	90	ALA	C-N-CA	-7.10	112.18	122.19
1	A	256	SER	N-CA-C	7.09	118.84	109.83
1	B	198	ARG	CD-NE-CZ	7.08	134.31	124.40
1	A	299	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	90	ALA	N-CA-CB	7.04	121.07	110.22
1	A	204	LEU	O-C-N	7.03	130.16	122.15
1	B	195	GLU	CA-C-O	7.02	127.86	120.42
1	A	208	ASP	CA-C-O	7.01	128.18	120.82
1	B	66	VAL	CA-C-N	-7.01	112.02	122.39
1	B	66	VAL	C-N-CA	-7.01	112.02	122.39
1	B	116	ARG	CG-CD-NE	-7.00	96.59	112.00
1	B	53	PRO	CA-C-O	-6.99	113.14	121.67
1	B	64	THR	O-C-N	6.99	131.53	123.29
1	B	48	ILE	O-C-N	-6.99	115.66	123.20
1	A	348	LEU	CA-C-O	-6.98	112.82	119.80
1	A	440	THR	N-CA-C	-6.98	103.67	111.28
1	B	158	ASN	CA-C-N	-6.98	113.28	123.05
1	B	158	ASN	C-N-CA	-6.98	113.28	123.05
1	A	249	GLN	CG-CD-NE2	6.98	126.87	116.40
1	A	428	VAL	CA-C-N	6.97	129.93	120.38
1	A	428	VAL	C-N-CA	6.97	129.93	120.38
1	A	48	ILE	O-C-N	-6.95	115.70	123.20
1	B	413	THR	CA-C-O	-6.94	112.69	120.32
1	A	39	ALA	CA-C-O	-6.92	113.05	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	GLU	CA-C-N	-6.92	111.03	120.44
1	B	434	GLU	C-N-CA	-6.92	111.03	120.44
1	A	376	MET	CA-C-O	6.91	127.88	119.38
1	B	450	GLN	N-CA-CB	-6.91	98.81	110.49
1	B	368	THR	CA-CB-CG2	6.91	122.25	110.50
1	B	11	LEU	CA-C-O	6.91	129.97	121.89
1	B	190	ARG	NE-CZ-NH1	-6.91	114.59	121.50
1	B	251	ALA	CA-C-O	6.89	128.14	120.70
1	A	137	GLY	CA-C-N	6.89	131.95	122.93
1	A	137	GLY	C-N-CA	6.89	131.95	122.93
1	A	167	LEU	CA-C-N	6.89	129.84	120.54
1	A	167	LEU	C-N-CA	6.89	129.84	120.54
1	B	410	ARG	NE-CZ-NH2	6.88	125.39	119.20
1	A	24	ARG	N-CA-CB	6.88	120.96	110.44
1	B	59	THR	CA-C-O	6.87	127.88	120.32
1	B	92	ILE	O-C-N	-6.87	115.92	123.20
1	A	332	GLU	O-C-N	6.87	127.98	121.38
1	B	250	GLY	N-CA-C	-6.87	99.95	111.08
1	A	45	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	416	ASN	CA-C-N	-6.86	111.74	122.51
1	A	416	ASN	C-N-CA	-6.86	111.74	122.51
1	A	203	TYR	CA-C-O	6.86	127.85	120.10
1	B	35	HIS	CA-C-O	-6.86	112.95	120.36
1	B	184	TRP	CG-CD2-CE3	-6.84	127.06	133.90
1	A	453	LYS	CA-CB-CG	6.83	127.75	114.10
1	B	149	ARG	NE-CZ-NH2	-6.82	113.06	119.20
1	B	428	VAL	O-C-N	-6.80	115.69	122.97
1	A	338	HIS	CG-CD2-NE2	-6.79	100.41	107.20
1	B	259	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	A	211	GLN	CA-C-O	-6.78	113.40	120.99
1	A	46	PHE	N-CA-C	6.78	120.03	109.52
1	A	382	LEU	CA-C-O	-6.77	111.74	120.00
1	A	91	ASP	CA-C-O	6.77	129.39	121.54
1	B	9	ILE	CA-CB-CG1	6.77	121.91	110.40
1	B	146	ASP	O-C-N	6.77	131.81	123.01
1	B	450	GLN	OE1-CD-NE2	6.76	129.37	122.60
1	B	430	ASP	CA-C-N	-6.76	108.35	121.06
1	B	430	ASP	C-N-CA	-6.76	108.35	121.06
1	A	435	ALA	CA-C-N	-6.76	109.44	120.72
1	A	435	ALA	C-N-CA	-6.76	109.44	120.72
1	A	350	GLU	CB-CG-CD	6.75	124.08	112.60
1	A	339	HIS	CA-C-N	-6.75	113.68	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	HIS	C-N-CA	-6.75	113.68	123.00
1	B	387	ARG	NH1-CZ-NH2	6.75	128.08	119.30
1	B	9	ILE	N-CA-CB	6.75	120.72	111.41
1	B	245	LEU	CA-C-O	-6.73	113.43	120.70
1	A	106	ALA	CA-C-O	-6.73	113.18	120.92
1	A	178	PHE	CA-C-O	6.73	128.55	120.81
1	A	218	PHE	O-C-N	-6.73	115.32	123.19
1	A	339	HIS	CE1-NE2-CD2	-6.72	102.28	109.00
1	A	327	GLU	CA-C-O	-6.69	112.31	120.54
1	B	97	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	A	311	ARG	NE-CZ-NH2	6.68	125.21	119.20
1	A	209	CYS	CB-CA-C	-6.67	97.10	110.30
1	B	169	SER	N-CA-C	6.66	120.67	112.54
1	B	198	ARG	CA-C-O	6.65	127.47	120.42
1	B	213	ASN	CA-CB-CG	-6.65	105.95	112.60
1	B	305	MET	CA-C-N	-6.65	109.39	120.30
1	B	305	MET	C-N-CA	-6.65	109.39	120.30
1	B	72	ARG	CA-C-N	-6.63	112.18	122.59
1	B	72	ARG	C-N-CA	-6.63	112.18	122.59
1	B	182	SER	O-C-N	-6.63	116.30	123.26
1	A	85	GLN	CA-C-N	6.63	129.15	120.60
1	A	85	GLN	C-N-CA	6.63	129.15	120.60
1	B	133	ASP	O-C-N	6.62	130.42	122.27
1	B	31	ALA	O-C-N	-6.62	115.29	123.04
1	B	257	PRO	CA-C-O	6.61	126.22	118.68
1	B	150	HIS	CA-CB-CG	-6.61	107.19	113.80
1	B	28	LEU	CB-CA-C	-6.61	99.86	109.38
1	B	134	MET	CA-C-O	-6.60	112.16	120.28
1	B	91	ASP	CA-C-N	-6.60	114.33	123.10
1	B	91	ASP	C-N-CA	-6.60	114.33	123.10
1	A	29	PRO	O-C-N	-6.60	114.51	122.89
1	B	114	LEU	CA-C-O	6.59	127.49	119.38
1	A	370	ALA	N-CA-C	6.58	124.36	109.81
1	B	446	ARG	CA-C-N	-6.58	112.14	120.56
1	B	446	ARG	C-N-CA	-6.58	112.14	120.56
1	A	449	LYS	CB-CG-CD	6.58	126.43	111.30
1	B	69	SER	CA-C-O	6.58	126.97	119.27
1	B	76	THR	O-C-N	-6.57	114.46	122.34
1	A	271	ARG	O-C-N	-6.56	115.50	121.34
1	B	267	GLU	CB-CG-CD	6.56	123.75	112.60
1	A	131	LEU	CB-CA-C	6.56	119.64	109.15
1	B	389	ALA	O-C-N	-6.55	113.88	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ASN	CA-C-O	6.54	129.13	121.54
1	A	358	LEU	CA-C-O	6.54	127.68	120.82
1	A	188	MET	CB-CA-C	-6.53	98.22	109.65
1	A	187	ASN	O-C-N	-6.53	111.91	122.42
1	A	338	HIS	CE1-NE2-CD2	6.51	115.51	109.00
1	B	299	ASP	CA-C-O	-6.50	110.52	119.16
1	B	172	PHE	CB-CA-C	-6.50	102.21	111.95
1	A	13	TRP	N-CA-C	6.49	119.89	110.28
1	B	172	PHE	CA-C-O	-6.48	114.44	122.03
1	A	227	TRP	CB-CG-CD2	6.47	135.86	126.80
1	B	19	GLU	CB-CG-CD	6.47	123.60	112.60
1	B	138	ILE	N-CA-CB	6.47	119.61	111.46
1	A	29	PRO	N-CD-CG	-6.47	93.50	103.20
1	A	347	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	B	427	ILE	CA-C-O	6.46	127.33	120.48
1	A	362	PHE	O-C-N	-6.46	112.85	121.64
1	A	6	PRO	CA-C-N	-6.46	112.18	121.42
1	A	6	PRO	C-N-CA	-6.46	112.18	121.42
1	A	74	THR	CA-CB-OG1	-6.46	99.91	109.60
1	B	183	ASP	CA-CB-CG	-6.46	106.14	112.60
1	B	175	GLN	CA-C-N	6.45	129.98	120.95
1	B	175	GLN	C-N-CA	6.45	129.98	120.95
1	B	256	SER	N-CA-C	6.45	118.02	109.83
1	B	444	VAL	O-C-N	6.44	130.62	122.57
1	B	161	ASN	O-C-N	6.43	128.70	122.07
1	B	270	THR	CA-C-O	-6.43	112.29	120.84
1	A	63	GLU	CA-C-O	-6.42	113.27	120.66
1	A	155	LEU	CA-C-O	-6.42	113.76	120.70
1	B	172	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	338	HIS	CA-C-N	-6.41	112.53	122.59
1	A	338	HIS	C-N-CA	-6.41	112.53	122.59
1	B	418	GLN	CA-C-N	-6.41	114.04	122.94
1	B	418	GLN	C-N-CA	-6.41	114.04	122.94
1	A	161	ASN	CA-CB-CG	6.40	119.00	112.60
1	B	178	PHE	N-CA-CB	6.40	119.87	109.95
1	B	249	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	A	146	ASP	CB-CA-C	-6.39	100.58	111.31
1	B	27	HIS	CA-C-N	-6.39	112.73	121.61
1	B	27	HIS	C-N-CA	-6.39	112.73	121.61
1	B	2	LYS	CA-CB-CG	6.38	126.86	114.10
1	B	200	VAL	CA-C-O	-6.38	113.88	120.71
1	B	393	SER	N-CA-C	6.38	119.41	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	TYR	CA-C-N	-6.38	109.84	120.68
1	B	437	TYR	C-N-CA	-6.38	109.84	120.68
1	A	309	LEU	CA-C-O	6.37	127.51	120.82
1	B	149	ARG	NH1-CZ-NH2	6.37	127.58	119.30
1	B	41	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	85	GLN	OE1-CD-NE2	-6.36	116.25	122.60
1	A	359	ARG	N-CA-C	6.35	119.01	111.71
1	A	76	THR	CA-CB-CG2	6.35	121.29	110.50
1	B	385	GLN	CA-C-N	6.34	129.88	120.87
1	B	385	GLN	C-N-CA	6.34	129.88	120.87
1	B	171	GLN	N-CA-C	6.34	118.19	111.28
1	B	146	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	351	GLN	OE1-CD-NE2	6.33	128.93	122.60
1	B	405	THR	CA-C-O	-6.33	114.50	121.33
1	A	387	ARG	CD-NE-CZ	-6.32	115.55	124.40
1	B	308	ASP	CA-CB-CG	-6.32	106.28	112.60
1	A	171	GLN	CA-C-N	6.30	132.42	122.34
1	A	171	GLN	C-N-CA	6.30	132.42	122.34
1	B	311	ARG	CA-C-O	-6.30	114.14	121.07
1	B	387	ARG	NE-CZ-NH1	-6.29	115.21	121.50
1	A	235	GLN	CA-C-O	6.29	127.43	120.82
1	A	71	LYS	CA-CB-CG	6.29	126.68	114.10
1	A	102	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	231	LEU	O-C-N	6.28	128.77	122.12
1	B	352	LEU	O-C-N	6.28	130.02	122.68
1	B	377	GLU	CA-C-O	6.27	127.07	120.42
1	B	370	ALA	CA-C-O	-6.27	113.26	120.03
1	A	15	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	A	195	GLU	CA-C-O	6.26	127.59	120.90
1	B	350	GLU	N-CA-C	6.25	120.01	112.38
1	A	209	CYS	O-C-N	6.25	131.50	122.94
1	B	135	ALA	CA-C-N	-6.25	114.31	122.99
1	B	135	ALA	C-N-CA	-6.25	114.31	122.99
1	B	67	SER	CA-C-N	6.25	133.69	122.64
1	B	67	SER	C-N-CA	6.25	133.69	122.64
1	A	234	ASN	CA-C-O	6.22	127.35	120.82
1	A	175	GLN	OE1-CD-NE2	6.21	128.81	122.60
1	A	208	ASP	O-C-N	-6.21	115.68	122.07
1	A	445	ASN	CA-C-O	-6.20	113.97	120.55
1	A	450	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	336	ALA	N-CA-CB	-6.18	100.78	110.30
1	B	354	ALA	CA-C-O	6.18	127.09	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ASN	O-C-N	6.17	130.37	122.10
1	A	94	PRO	CB-CA-C	-6.17	102.90	110.98
1	B	38	TYR	CA-CB-CG	-6.17	102.80	113.90
1	A	98	GLU	CA-C-N	-6.17	111.22	122.38
1	A	98	GLU	C-N-CA	-6.17	111.22	122.38
1	A	168	GLU	CA-C-N	6.17	131.02	120.72
1	A	168	GLU	C-N-CA	6.17	131.02	120.72
1	A	446	ARG	O-C-N	6.16	130.68	122.43
1	A	359	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	445	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	B	153	SER	CA-C-O	-6.16	113.67	120.38
1	A	390	TRP	CB-CG-CD2	-6.15	118.19	126.80
1	A	127	GLN	OE1-CD-NE2	-6.14	116.45	122.60
1	A	164	ARG	CA-C-N	6.14	128.42	120.44
1	A	164	ARG	C-N-CA	6.14	128.42	120.44
1	A	340	LEU	CA-C-O	-6.14	113.69	120.38
1	B	122	PRO	O-C-N	-6.14	115.48	122.91
1	B	266	SER	O-C-N	6.13	128.31	121.87
1	B	439	GLU	CA-CB-CG	6.13	126.36	114.10
1	A	27	HIS	CA-C-O	6.13	126.52	119.35
1	A	312	ASN	O-C-N	6.13	129.14	122.15
1	A	183	ASP	N-CA-CB	6.13	119.20	110.44
1	B	196	LYS	CD-CE-NZ	-6.13	92.29	111.90
1	B	412	LEU	CA-C-N	-6.12	114.49	123.05
1	B	412	LEU	C-N-CA	-6.12	114.49	123.05
1	B	36	SER	CA-C-N	6.11	129.34	120.11
1	B	36	SER	C-N-CA	6.11	129.34	120.11
1	B	379	ILE	CA-C-O	6.11	127.33	120.85
1	A	369	GLY	CA-C-N	6.11	136.71	121.80
1	A	369	GLY	C-N-CA	6.11	136.71	121.80
1	B	3	THR	N-CA-CB	-6.11	101.60	110.70
1	A	84	GLN	CA-C-N	-6.10	112.14	120.44
1	A	84	GLN	C-N-CA	-6.10	112.14	120.44
1	A	161	ASN	N-CA-CB	6.10	119.64	110.19
1	B	175	GLN	CA-C-O	-6.10	111.79	120.51
1	B	12	LEU	O-C-N	-6.09	115.40	122.95
1	B	269	GLN	OE1-CD-NE2	6.08	128.68	122.60
1	B	164	ARG	N-CA-CB	6.07	119.05	110.12
1	B	224	GLY	CA-C-N	6.07	131.03	121.99
1	B	224	GLY	C-N-CA	6.07	131.03	121.99
1	A	266	SER	CA-C-O	6.06	127.53	119.59
1	A	407	ILE	N-CA-C	-6.06	99.01	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	GLN	CA-C-O	-6.05	113.60	120.32
1	B	259	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	A	179	THR	CA-C-O	-6.05	113.34	120.60
1	A	172	PHE	CB-CA-C	-6.05	101.52	111.68
1	B	27	HIS	CA-C-O	6.03	126.41	119.35
1	A	146	ASP	O-C-N	6.03	130.29	122.87
1	A	372	LYS	N-CA-C	6.03	118.34	111.11
1	A	164	ARG	O-C-N	6.02	129.01	122.15
1	A	365	GLY	CA-C-N	-6.02	110.67	120.72
1	A	365	GLY	C-N-CA	-6.02	110.67	120.72
1	B	28	LEU	N-CA-C	6.01	117.60	109.24
1	B	170	GLN	CA-CB-CG	-6.01	102.08	114.10
1	B	39	ALA	CA-C-O	6.01	127.54	120.69
1	A	215	ALA	O-C-N	6.00	130.95	123.15
1	A	138	ILE	CA-C-N	5.99	131.44	123.05
1	A	138	ILE	C-N-CA	5.99	131.44	123.05
1	B	263	CYS	CA-C-N	5.99	131.17	122.85
1	B	263	CYS	C-N-CA	5.99	131.17	122.85
1	B	126	GLU	CA-C-O	5.98	128.54	121.36
1	A	5	SER	CA-CB-OG	-5.98	99.14	111.10
1	B	127	GLN	CB-CG-CD	-5.98	102.43	112.60
1	A	80	LEU	O-C-N	5.97	130.34	122.33
1	A	52	GLU	O-C-N	-5.97	114.45	121.32
1	B	175	GLN	CA-CB-CG	5.97	126.04	114.10
1	B	3	THR	CA-C-N	-5.96	108.70	121.45
1	B	3	THR	C-N-CA	-5.96	108.70	121.45
1	B	13	TRP	CA-C-O	5.96	127.83	121.16
1	B	202	GLU	CA-C-N	5.96	128.26	120.28
1	B	202	GLU	C-N-CA	5.96	128.26	120.28
1	B	72	ARG	O-C-N	-5.94	116.23	123.30
1	A	307	VAL	O-C-N	-5.94	116.09	121.91
1	A	107	LEU	CB-CA-C	5.93	121.43	109.68
1	A	188	MET	N-CA-C	5.93	119.19	108.69
1	A	316	ARG	CA-C-O	5.93	126.70	119.11
1	B	366	SER	CA-C-N	-5.93	112.44	122.88
1	B	366	SER	C-N-CA	-5.93	112.44	122.88
1	A	115	GLY	O-C-N	-5.92	116.10	122.19
1	A	323	VAL	N-CA-CB	-5.92	104.08	110.53
1	A	186	SER	O-C-N	5.91	129.59	122.85
1	B	31	ALA	N-CA-CB	5.91	119.11	109.95
1	B	116	ARG	O-C-N	-5.91	114.57	122.43
1	B	401	GLY	O-C-N	-5.91	115.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	VAL	CA-CB-CG1	-5.90	100.37	110.40
1	A	341	VAL	N-CA-C	5.90	117.94	108.85
1	B	198	ARG	NE-CZ-NH1	5.90	127.40	121.50
1	A	333	PRO	CA-C-O	5.90	131.34	120.60
1	B	221	THR	CB-CA-C	5.90	119.53	109.80
1	B	375	ALA	CA-C-N	-5.88	110.89	120.72
1	B	375	ALA	C-N-CA	-5.88	110.89	120.72
1	A	354	ALA	CA-C-N	-5.88	111.81	120.28
1	A	354	ALA	C-N-CA	-5.88	111.81	120.28
1	A	259	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	B	148	GLN	CA-C-O	-5.88	112.83	120.00
1	B	54	ILE	CA-CB-CG2	-5.88	100.51	110.50
1	B	83	LEU	CB-CA-C	-5.88	101.03	110.79
1	B	361	ALA	N-CA-C	5.88	121.36	113.72
1	A	380	ASP	CA-C-N	-5.87	110.54	120.58
1	A	380	ASP	C-N-CA	-5.87	110.54	120.58
1	B	428	VAL	CA-C-N	5.87	132.75	121.54
1	B	428	VAL	C-N-CA	5.87	132.75	121.54
1	A	392	GLY	O-C-N	-5.86	114.89	122.80
1	B	29	PRO	O-C-N	-5.86	115.70	122.85
1	B	93	ARG	CD-NE-CZ	5.86	132.60	124.40
1	B	104	GLY	O-C-N	-5.86	115.87	122.78
1	A	73	THR	CA-C-O	-5.85	114.61	121.46
1	A	257	PRO	N-CA-C	-5.85	107.19	114.68
1	A	46	PHE	CB-CA-C	-5.85	97.81	109.79
1	A	420	PHE	CE1-CZ-CE2	-5.83	109.50	120.00
1	B	102	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	431	SER	O-C-N	5.83	129.77	122.65
1	A	38	TYR	O-C-N	-5.83	114.76	122.40
1	A	53	PRO	CA-C-O	-5.83	114.56	121.67
1	B	166	TRP	CD2-CE3-CZ3	-5.83	111.03	118.60
1	B	386	ARG	O-C-N	5.82	129.99	122.89
1	A	52	GLU	CB-CG-CD	-5.82	102.71	112.60
1	A	323	VAL	O-C-N	-5.81	116.36	122.81
1	B	422	SER	CA-C-O	5.81	128.59	121.56
1	A	39	ALA	CA-C-N	5.80	130.94	122.41
1	A	39	ALA	C-N-CA	5.80	130.94	122.41
1	A	428	VAL	O-C-N	-5.80	116.83	122.92
1	B	133	ASP	N-CA-C	-5.80	105.09	111.82
1	B	256	SER	CB-CA-C	-5.80	100.32	109.42
1	A	450	GLN	CA-C-O	5.80	126.51	119.38
1	A	160	VAL	O-C-N	5.78	130.18	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	GLU	O-C-N	5.78	128.74	122.15
1	B	208	ASP	N-CA-C	-5.78	104.62	111.03
1	A	141	TRP	CA-C-O	-5.77	115.28	121.45
1	B	208	ASP	CA-C-N	5.77	131.56	122.21
1	B	208	ASP	C-N-CA	5.77	131.56	122.21
1	A	126	GLU	O-C-N	-5.76	115.86	122.89
1	B	259	ARG	O-C-N	-5.76	116.06	122.86
1	B	305	MET	N-CA-CB	5.76	118.69	110.16
1	B	386	ARG	CA-C-O	-5.76	114.70	121.16
1	A	270	THR	O-C-N	-5.76	116.33	123.36
1	B	89	ARG	N-CA-C	5.75	119.39	112.38
1	B	54	ILE	CA-CB-CG1	5.74	120.17	110.40
1	B	249	GLN	CA-C-N	-5.74	113.50	120.51
1	B	249	GLN	C-N-CA	-5.74	113.50	120.51
1	A	19	GLU	CA-CB-CG	-5.74	102.62	114.10
1	A	438	GLN	CA-C-O	5.74	126.44	119.38
1	B	162	ALA	CA-C-N	-5.74	112.59	120.28
1	B	162	ALA	C-N-CA	-5.74	112.59	120.28
1	A	249	GLN	CA-C-N	-5.73	113.09	120.72
1	A	249	GLN	C-N-CA	-5.73	113.09	120.72
1	A	199	GLN	CB-CG-CD	-5.73	102.85	112.60
1	A	377	GLU	O-C-N	5.73	128.68	122.15
1	A	47	ASP	N-CA-C	-5.72	99.68	109.24
1	B	169	SER	CA-C-N	5.72	132.47	121.54
1	B	169	SER	C-N-CA	5.72	132.47	121.54
1	A	43	TYR	CA-C-N	-5.72	112.10	122.50
1	A	43	TYR	C-N-CA	-5.72	112.10	122.50
1	B	237	ASN	CA-C-N	-5.72	114.24	122.36
1	B	237	ASN	C-N-CA	-5.72	114.24	122.36
1	B	230	PHE	CA-C-N	5.71	127.93	120.28
1	B	230	PHE	C-N-CA	5.71	127.93	120.28
1	A	144	ILE	CB-CA-C	-5.71	102.66	110.77
1	A	422	SER	CA-C-O	-5.71	114.47	121.78
1	B	223	SER	CA-CB-OG	-5.71	99.69	111.10
1	A	62	LYS	CG-CD-CE	5.70	124.41	111.30
1	A	232	GLN	CG-CD-NE2	5.69	124.94	116.40
1	B	5	SER	CA-C-N	-5.69	114.73	120.31
1	B	5	SER	C-N-CA	-5.69	114.73	120.31
1	B	81	GLN	CA-C-O	5.69	126.45	120.42
1	B	357	LEU	CA-C-O	5.68	126.50	119.97
1	A	161	ASN	N-CA-C	-5.68	103.86	112.04
1	A	51	ALA	O-C-N	5.67	128.59	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	PHE	CA-C-O	-5.66	114.24	120.24
1	A	196	LYS	CA-C-O	-5.66	113.11	119.79
1	A	358	LEU	N-CA-C	-5.66	105.01	111.07
1	A	403	MET	CA-C-O	-5.66	114.65	120.99
1	A	166	TRP	CE3-CZ3-CH2	5.66	128.45	121.10
1	A	303	ASN	N-CA-CB	-5.66	101.81	110.01
1	B	184	TRP	CE2-CD2-CE3	5.65	124.45	118.80
1	A	153	SER	CA-C-O	5.65	126.46	120.36
1	B	148	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	B	407	ILE	N-CA-C	-5.65	100.28	108.36
1	A	239	ALA	CB-CA-C	5.65	117.50	109.08
1	B	4	LEU	N-CA-C	5.64	117.81	110.53
1	B	42	PRO	CA-C-O	5.64	126.36	118.86
1	A	43	TYR	O-C-N	5.64	130.09	122.59
1	A	159	ASP	O-C-N	-5.64	116.03	123.13
1	A	250	GLY	N-CA-C	-5.64	103.02	110.74
1	A	129	ILE	CA-C-N	5.63	126.94	121.65
1	A	129	ILE	C-N-CA	5.63	126.94	121.65
1	A	138	ILE	N-CA-CB	5.63	118.45	111.41
1	A	258	GLU	N-CA-C	5.63	117.70	108.52
1	A	56	THR	CA-CB-OG1	-5.63	101.16	109.60
1	A	134	MET	N-CA-CB	5.63	119.94	110.77
1	B	200	VAL	O-C-N	5.62	129.26	121.84
1	B	404	ASP	N-CA-C	-5.62	99.14	108.75
1	A	318	ALA	O-C-N	5.62	129.51	122.65
1	B	35	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	308	ASP	CA-C-N	5.61	127.73	120.44
1	A	308	ASP	C-N-CA	5.61	127.73	120.44
1	B	252	ILE	O-C-N	-5.61	116.54	123.10
1	B	60	PHE	CG-CD2-CE2	-5.60	111.17	120.70
1	A	390	TRP	CB-CG-CD1	5.60	135.30	126.90
1	A	235	GLN	CB-CG-CD	5.60	122.12	112.60
1	A	433	GLU	CA-C-N	-5.60	111.00	120.58
1	A	433	GLU	C-N-CA	-5.60	111.00	120.58
1	A	58	THR	CA-CB-OG1	-5.60	101.20	109.60
1	B	215	ALA	N-CA-C	5.59	118.66	109.72
1	A	40	ASP	N-CA-C	-5.58	98.16	107.99
1	B	323	VAL	CB-CA-C	-5.58	105.20	111.23
1	B	297	ALA	O-C-N	5.58	131.92	123.00
1	A	95	THR	CA-C-N	5.57	128.76	120.90
1	A	95	THR	C-N-CA	5.57	128.76	120.90
1	A	157	HIS	CA-CB-CG	-5.57	108.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLU	CA-C-N	5.57	128.68	120.82
1	A	176	GLU	C-N-CA	5.57	128.68	120.82
1	B	322	SER	N-CA-C	-5.57	106.47	113.72
1	A	167	LEU	CB-CA-C	-5.57	101.21	110.68
1	A	109	LEU	N-CA-C	5.57	118.32	109.24
1	B	216	GLN	CB-CG-CD	-5.57	103.13	112.60
1	A	448	LEU	CA-C-O	5.56	126.31	120.42
1	A	224	GLY	CA-C-N	5.55	130.31	122.09
1	A	224	GLY	C-N-CA	5.55	130.31	122.09
1	B	430	ASP	N-CA-C	5.55	119.36	112.59
1	A	56	THR	O-C-N	-5.54	115.94	123.15
1	A	22	PHE	CA-C-O	-5.54	114.55	120.42
1	A	117	ARG	NH1-CZ-NH2	5.54	126.50	119.30
1	A	451	LEU	CA-C-O	5.54	126.17	119.31
1	A	106	ALA	O-C-N	5.53	129.58	123.16
1	B	418	GLN	CG-CD-NE2	-5.53	108.10	116.40
1	A	130	VAL	CA-C-O	-5.53	117.82	122.63
1	A	202	GLU	O-C-N	5.53	128.45	122.15
1	A	395	GLY	N-CA-C	-5.53	103.33	110.69
1	B	246	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	B	156	SER	CA-CB-OG	5.52	122.14	111.10
1	B	388	ASN	O-C-N	-5.52	112.56	121.23
1	A	21	TYR	CB-CG-CD1	-5.51	112.53	120.80
1	A	175	GLN	CG-CD-OE1	-5.51	109.77	120.80
1	B	299	ASP	O-C-N	5.51	127.66	121.87
1	B	16	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	133	ASP	CA-C-O	-5.51	113.64	119.97
1	A	118	PHE	O-C-N	-5.50	115.58	122.35
1	A	277	LEU	CA-C-N	-5.50	114.58	120.03
1	A	277	LEU	C-N-CA	-5.50	114.58	120.03
1	A	17	ALA	N-CA-C	5.50	118.03	111.71
1	A	323	VAL	N-CA-C	5.50	116.14	108.89
1	B	44	SER	CA-C-N	-5.49	111.54	120.71
1	B	44	SER	C-N-CA	-5.49	111.54	120.71
1	A	251	ALA	CA-C-N	-5.49	116.38	123.19
1	A	251	ALA	C-N-CA	-5.49	116.38	123.19
1	A	339	HIS	ND1-CG-CD2	-5.49	100.61	106.10
1	B	50	VAL	CA-C-O	-5.49	115.46	121.28
1	B	46	PHE	CA-C-N	5.48	130.88	122.93
1	B	46	PHE	C-N-CA	5.48	130.88	122.93
1	A	294	ALA	CA-C-N	5.48	130.99	122.49
1	A	294	ALA	C-N-CA	5.48	130.99	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	LEU	CA-C-N	5.48	132.01	121.54
1	B	204	LEU	C-N-CA	5.48	132.01	121.54
1	A	311	ARG	NH1-CZ-NH2	-5.47	112.18	119.30
1	B	270	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	203	TYR	O-C-N	5.47	127.92	122.12
1	A	25	LEU	O-C-N	5.47	129.82	122.49
1	B	161	ASN	CB-CA-C	-5.47	102.29	110.88
1	A	110	PHE	O-C-N	-5.47	114.65	122.96
1	B	157	HIS	N-CA-C	-5.47	106.61	113.28
1	A	332	GLU	CA-C-N	5.46	126.67	119.84
1	A	332	GLU	C-N-CA	5.46	126.67	119.84
1	B	32	MET	CA-C-O	-5.46	114.05	120.60
1	B	368	THR	CA-C-N	5.46	132.10	121.41
1	B	368	THR	C-N-CA	5.46	132.10	121.41
1	A	232	GLN	CB-CG-CD	5.45	121.86	112.60
1	A	188	MET	CA-C-O	-5.45	113.58	120.28
1	B	237	ASN	CA-CB-CG	-5.45	107.15	112.60
1	B	270	THR	O-C-N	5.45	128.92	121.78
1	B	437	TYR	CA-C-O	5.45	126.51	120.63
1	A	373	VAL	N-CA-C	5.44	116.17	110.62
1	B	307	VAL	CA-C-N	-5.44	112.04	120.31
1	B	307	VAL	C-N-CA	-5.44	112.04	120.31
1	A	55	CYS	CA-C-O	-5.44	113.85	120.54
1	A	317	VAL	N-CA-CB	-5.44	102.26	111.23
1	B	2	LYS	N-CA-CB	-5.44	101.35	110.65
1	A	238	ARG	CD-NE-CZ	5.44	132.01	124.40
1	B	417	GLY	CA-C-O	-5.44	113.62	119.27
1	B	351	GLN	CG-CD-OE1	5.43	131.66	120.80
1	B	90	ALA	N-CA-C	-5.42	105.47	111.71
1	B	407	ILE	N-CA-CB	5.42	117.49	110.99
1	A	134	MET	CA-C-O	-5.41	113.60	120.20
1	B	159	ASP	CA-CB-CG	5.41	118.00	112.60
1	B	397	LEU	CA-C-N	5.41	128.55	120.87
1	B	397	LEU	C-N-CA	5.41	128.55	120.87
1	B	238	ARG	N-CA-CB	-5.40	103.71	111.70
1	B	85	GLN	CA-C-O	5.40	126.27	120.55
1	B	244	PHE	CB-CG-CD1	5.40	129.88	120.70
1	B	450	GLN	CA-C-O	5.40	128.23	120.51
1	B	235	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	38	TYR	N-CA-C	-5.39	104.21	111.54
1	B	119	GLU	CA-C-O	-5.39	112.72	120.11
1	B	327	GLU	CA-C-O	5.38	129.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ILE	N-CA-CB	-5.38	105.12	112.28
1	A	415	ILE	CA-CB-CG1	5.38	119.55	110.40
1	B	441	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	256	SER	CA-C-O	-5.38	114.44	120.25
1	A	233	LEU	O-C-N	-5.37	116.42	122.12
1	B	89	ARG	CA-C-N	5.37	128.02	120.28
1	B	89	ARG	C-N-CA	5.37	128.02	120.28
1	B	197	PHE	N-CA-C	-5.37	105.42	111.28
1	B	317	VAL	N-CA-C	5.36	118.78	113.53
1	B	447	ILE	CB-CA-C	-5.36	105.00	112.02
1	A	364	GLY	O-C-N	5.36	129.66	122.70
1	B	168	GLU	CA-C-O	5.36	126.23	120.55
1	A	55	CYS	CA-C-N	-5.35	114.19	122.59
1	A	55	CYS	C-N-CA	-5.35	114.19	122.59
1	B	184	TRP	CB-CG-CD2	-5.35	119.31	126.80
1	B	374	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	310	MET	O-C-N	5.35	127.58	122.07
1	A	188	MET	O-C-N	5.34	129.88	123.36
1	A	350	GLU	CA-C-O	-5.34	113.03	119.49
1	A	70	GLU	N-CA-CB	-5.34	102.45	110.73
1	B	95	THR	CA-CB-OG1	-5.34	101.60	109.60
1	A	72	ARG	CG-CD-NE	5.33	123.73	112.00
1	A	274	LYS	O-C-N	5.33	130.28	123.24
1	A	217	ARG	O-C-N	5.33	129.55	123.31
1	B	37	GLY	CA-C-N	5.33	132.76	123.91
1	B	37	GLY	C-N-CA	5.33	132.76	123.91
1	B	127	GLN	CG-CD-OE1	-5.33	110.14	120.80
1	A	62	LYS	N-CA-C	5.32	119.53	113.19
1	B	385	GLN	O-C-N	5.32	130.24	123.11
1	B	56	THR	CA-CB-CG2	5.32	119.55	110.50
1	A	427	ILE	O-C-N	5.32	129.01	123.26
1	B	128	ASP	CA-C-O	-5.32	112.86	119.18
1	A	3	THR	CA-C-O	5.31	129.83	120.80
1	A	212	VAL	CA-C-O	-5.31	114.96	120.64
1	B	188	MET	O-C-N	-5.31	116.79	123.27
1	B	133	ASP	CA-CB-CG	-5.31	107.29	112.60
1	B	246	ARG	CA-C-O	-5.30	115.02	120.54
1	A	276	THR	OG1-CB-CG2	-5.30	98.70	109.30
1	A	141	TRP	O-C-N	5.29	129.19	123.10
1	A	116	ARG	CA-C-O	-5.29	113.09	119.49
1	B	161	ASN	N-CA-C	5.29	116.73	111.07
1	A	157	HIS	N-CA-CB	5.28	118.68	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLN	N-CA-CB	5.28	117.98	110.16
1	A	3	THR	OG1-CB-CG2	-5.28	98.74	109.30
1	A	97	ASN	O-C-N	5.28	130.21	123.24
1	B	255	LEU	O-C-N	-5.28	114.85	121.97
1	A	53	PRO	O-C-N	5.27	129.55	123.06
1	A	441	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	37	GLY	CA-C-O	-5.27	113.00	119.69
1	B	416	ASN	CB-CA-C	-5.26	103.80	112.06
1	A	168	GLU	N-CA-C	5.26	117.42	111.11
1	B	43	TYR	CB-CA-C	-5.26	101.91	110.85
1	B	391	CYS	CA-CB-SG	-5.25	102.31	114.40
1	A	246	ARG	N-CA-C	-5.25	99.23	108.20
1	B	234	ASN	CA-C-N	-5.25	112.34	120.31
1	B	234	ASN	C-N-CA	-5.25	112.34	120.31
1	A	366	SER	CA-C-O	5.24	125.83	119.38
1	B	347	GLN	CA-C-O	5.24	127.66	121.58
1	A	261	ILE	CB-CG1-CD1	5.24	124.79	113.80
1	A	443	LYS	CA-C-N	-5.23	112.56	121.97
1	A	443	LYS	C-N-CA	-5.23	112.56	121.97
1	B	375	ALA	CA-C-O	5.23	126.09	120.55
1	B	237	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	193	TYR	CB-CG-CD1	5.21	128.62	120.80
1	B	444	VAL	CA-C-O	-5.21	114.26	120.78
1	A	58	THR	CA-C-O	-5.21	114.72	120.24
1	A	116	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	A	373	VAL	CA-C-O	-5.20	115.54	120.95
1	B	49	VAL	O-C-N	5.20	128.87	123.26
1	B	193	TYR	CG-CD1-CE1	5.20	128.99	121.20
1	A	97	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	439	GLU	CB-CG-CD	5.19	121.43	112.60
1	B	396	TYR	CB-CG-CD1	5.19	128.59	120.80
1	A	65	VAL	O-C-N	5.19	129.17	123.10
1	A	158	ASN	CA-CB-CG	-5.19	107.41	112.60
1	B	245	LEU	CA-C-N	-5.19	116.10	122.84
1	B	245	LEU	C-N-CA	-5.19	116.10	122.84
1	B	217	ARG	CA-C-O	-5.18	114.75	120.30
1	A	383	GLU	CA-C-O	5.18	124.62	119.49
1	A	213	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	3	THR	CA-C-N	5.18	131.43	121.54
1	A	3	THR	C-N-CA	5.18	131.43	121.54
1	B	351	GLN	O-C-N	5.18	129.20	122.42
1	A	75	THR	CA-C-O	5.17	126.53	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ILE	CB-CG1-CD1	-5.17	102.94	113.80
1	A	303	ASN	O-C-N	-5.17	116.75	122.07
1	B	434	GLU	CA-C-O	5.17	125.94	120.10
1	A	166	TRP	CD2-CE2-CZ2	5.17	127.57	122.40
1	B	168	GLU	O-C-N	-5.17	116.64	122.12
1	B	126	GLU	N-CA-C	5.17	118.53	110.32
1	B	311	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
1	B	316	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	321	GLY	N-CA-C	-5.16	100.95	113.18
1	B	428	VAL	CA-C-O	5.16	127.84	121.75
1	A	64	THR	O-C-N	5.15	129.43	123.30
1	A	366	SER	O-C-N	-5.15	115.53	122.43
1	A	433	GLU	CA-C-O	5.15	126.41	120.90
1	B	23	SER	CA-C-N	-5.14	110.99	121.18
1	B	23	SER	C-N-CA	-5.14	110.99	121.18
1	A	10	THR	CB-CA-C	5.14	118.01	109.53
1	B	371	PRO	N-CA-CB	5.14	108.25	102.60
1	A	216	GLN	O-C-N	5.14	129.73	123.10
1	B	91	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	347	GLN	O-C-N	5.12	129.31	123.31
1	B	198	ARG	N-CA-C	-5.12	105.77	111.36
1	B	322	SER	CA-C-O	5.12	124.69	119.05
1	A	294	ALA	CA-C-O	5.12	129.51	120.80
1	B	318	ALA	N-CA-C	5.12	117.29	110.53
1	B	427	ILE	CB-CG1-CD1	-5.12	103.05	113.80
1	A	239	ALA	CA-C-N	5.12	124.83	119.82
1	A	239	ALA	C-N-CA	5.12	124.83	119.82
1	B	15	GLN	CA-C-N	-5.11	114.95	122.83
1	B	15	GLN	C-N-CA	-5.11	114.95	122.83
1	B	424	GLY	CA-C-O	-5.11	115.74	121.31
1	B	234	ASN	CB-CG-ND2	5.11	124.06	116.40
1	A	60	PHE	N-CA-CB	5.11	118.72	110.65
1	B	313	ASP	N-CA-C	-5.11	104.79	111.02
1	B	155	LEU	CD1-CG-CD2	-5.10	99.57	110.80
1	A	225	ASP	CA-C-O	5.10	126.79	120.92
1	B	125	ALA	O-C-N	-5.10	116.54	122.81
1	A	217	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	B	305	MET	N-CA-C	-5.10	105.81	111.36
1	A	368	THR	O-C-N	-5.09	115.30	121.92
1	B	319	VAL	CA-CB-CG1	5.09	119.06	110.40
1	A	166	TRP	CB-CG-CD1	-5.09	119.27	126.90
1	A	279	ARG	NE-CZ-NH2	5.09	123.78	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	B	196	LYS	CA-C-N	5.08	127.09	120.28
1	B	196	LYS	C-N-CA	5.08	127.09	120.28
1	B	368	THR	N-CA-CB	-5.08	101.91	110.49
1	B	9	ILE	CB-CA-C	-5.08	103.12	110.63
1	B	258	GLU	CB-CA-C	-5.08	100.24	109.38
1	A	422	SER	O-C-N	5.07	130.02	122.97
1	B	35	HIS	CG-CD2-NE2	5.07	112.27	107.20
1	B	346	ALA	O-C-N	-5.07	115.85	122.59
1	B	225	ASP	CB-CA-C	-5.07	102.31	110.77
1	B	130	VAL	N-CA-CB	-5.07	107.15	112.06
1	B	181	THR	O-C-N	-5.06	115.64	122.22
1	B	201	GLN	O-C-N	-5.06	116.75	122.12
1	B	44	SER	CA-CB-OG	5.06	121.22	111.10
1	A	98	GLU	O-C-N	-5.06	115.75	122.33
1	A	322	SER	O-C-N	-5.06	115.04	122.43
1	B	402	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	B	37	GLY	N-CA-C	5.05	120.86	113.48
1	A	387	ARG	NH1-CZ-NH2	-5.05	112.74	119.30
1	B	243	ALA	N-CA-C	5.05	116.74	108.76
1	A	168	GLU	CA-C-O	5.04	126.30	120.90
1	B	148	GLN	O-C-N	5.04	129.69	122.28
1	B	76	THR	CA-C-O	5.04	125.46	119.56
1	B	149	ARG	CA-C-O	-5.04	113.19	119.18
1	A	416	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	176	GLU	CB-CG-CD	5.03	121.16	112.60
1	B	222	TYR	CB-CG-CD2	5.03	128.35	120.80
1	B	167	LEU	CA-C-O	-5.02	115.53	120.90
1	B	3	THR	CB-CA-C	5.02	119.30	110.36
1	A	90	ALA	O-C-N	5.02	129.38	122.46
1	A	17	ALA	CA-C-O	-5.02	114.43	120.10
1	A	66	VAL	CA-C-N	-5.01	115.02	122.74
1	A	66	VAL	C-N-CA	-5.01	115.02	122.74
1	A	202	GLU	CA-C-O	-5.01	115.11	120.42
1	A	360	ALA	CA-C-N	-5.01	114.73	122.49
1	A	360	ALA	C-N-CA	-5.01	114.73	122.49
1	B	239	ALA	CA-C-N	5.01	124.67	119.56
1	B	239	ALA	C-N-CA	5.01	124.67	119.56
1	B	307	VAL	CA-CB-CG1	-5.00	101.89	110.40
1	B	427	ILE	CA-CB-CG2	5.00	119.01	110.50
1	A	259	ARG	CA-C-O	-5.00	114.99	120.69
1	A	399	PHE	N-CA-CB	5.00	117.92	110.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3466	0	3370	111	0
1	B	3289	0	3192	129	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
3	A	3	0	2	4	0
4	A	186	0	0	10	0
4	B	132	0	0	5	0
All	All	7106	0	6582	240	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 18.

All (240) 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)
1:B:225:ASP:HB3	1:B:228:GLN:HG2	1.40	0.99
1:A:176:GLU:HG3	1:A:224:GLY:HA2	1.45	0.95
1:B:114:LEU:HD21	1:B:134:MET:HE3	1.49	0.92
1:B:121:LEU:HD11	1:B:376:MET:HE3	1.53	0.90
1:B:176:GLU:HB2	1:B:225:ASP:HB2	1.56	0.84
1:A:236:ALA:HB1	1:A:446:ARG:HH22	1.40	0.84
1:B:300:ARG:HA	1:B:303:ASN:HD21	1.43	0.83
1:A:423:ALA:HA	3:A:1701:FMT:H	1.61	0.83
1:B:307:VAL:HG12	1:B:311:ARG:HH12	1.45	0.80
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.46	0.80
1:B:368:THR:HG21	1:B:372:LYS:HG3	1.63	0.80
1:B:311:ARG:HB2	1:B:311:ARG:HH11	1.48	0.78
1:B:177:ASP:O	1:B:224:GLY:HA3	1.83	0.78
1:A:40:ASP:H	1:A:238:ARG:NH2	1.84	0.76
1:A:446:ARG:HG2	1:A:449:LYS:HE3	1.67	0.76
1:A:208:ASP:HB3	1:A:374:ARG:HE	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:O	1:B:415:ILE:HG13	1.84	0.74
1:B:381:GLU:HG2	1:B:382:LEU:HD23	1.68	0.74
1:B:367:ILE:HD13	1:B:391:CYS:HB3	1.67	0.73
1:B:35:HIS:HD2	1:B:37:GLY:H	1.36	0.73
1:B:446:ARG:O	1:B:450:GLN:HB2	1.88	0.73
1:A:188:MET:HE2	1:A:216:GLN:HB3	1.69	0.72
1:B:299:ASP:HA	1:B:302:GLU:HB2	1.72	0.71
1:B:300:ARG:O	1:B:304:LEU:HG	1.90	0.71
1:A:296:SER:O	1:A:300:ARG:HG2	1.89	0.71
1:A:273:ILE:HG12	1:A:341:VAL:HG22	1.72	0.71
1:B:1:MET:HG3	1:B:2:LYS:HB3	1.71	0.71
1:A:424:GLY:H	3:A:1701:FMT:H	1.57	0.70
1:B:36:SER:HG	2:B:602:TRP:N	1.90	0.70
1:B:113:ASP:HB2	4:B:1188:HOH:O	1.93	0.69
1:B:170:GLN:NE2	1:B:172:PHE:HB3	2.07	0.68
1:A:35:HIS:HD2	1:A:37:GLY:H	1.39	0.68
1:B:307:VAL:HG12	1:B:311:ARG:NH1	2.08	0.67
1:B:269:GLN:NE2	1:B:343:THR:HG21	2.09	0.67
1:B:9:ILE:HD12	1:B:160:VAL:HG22	1.77	0.67
1:B:41:HIS:HB2	1:B:44:SER:OG	1.94	0.67
1:A:23:SER:HB3	1:A:172:PHE:CD1	2.30	0.66
1:B:267:GLU:O	1:B:267:GLU:HG3	1.96	0.66
1:A:99:ASP:HB3	1:A:149:ARG:HH21	1.61	0.65
1:B:450:GLN:HG2	4:B:1280:HOH:O	1.97	0.64
1:B:303:ASN:HA	1:B:306:ILE:HG13	1.79	0.64
1:A:40:ASP:H	1:A:238:ARG:HH22	1.45	0.64
1:A:183:ASP:HB3	4:A:1097:HOH:O	1.98	0.63
1:A:41:HIS:HB3	1:A:44:SER:HB3	1.81	0.63
1:A:3:THR:HG23	1:A:4:LEU:HD12	1.81	0.62
1:B:3:THR:HG21	1:B:93:ARG:H	1.63	0.62
1:B:308:ASP:HA	1:B:311:ARG:NH1	2.15	0.62
1:B:307:VAL:HG13	1:B:344:ILE:HD11	1.82	0.62
1:B:303:ASN:O	1:B:306:ILE:HG13	2.00	0.61
1:A:208:ASP:CB	1:A:374:ARG:HE	2.14	0.60
1:B:159:ASP:OD1	1:B:161:ASN:HB2	2.01	0.60
1:B:297:ALA:O	1:B:300:ARG:HG3	2.02	0.60
1:B:4:LEU:H	1:B:4:LEU:HD23	1.66	0.60
1:B:198:ARG:O	1:B:202:GLU:HG3	2.01	0.59
1:A:89:ARG:O	1:A:89:ARG:HG2	2.02	0.59
1:A:69:SER:HB2	1:A:70:GLU:HG3	1.85	0.58
1:B:121:LEU:HD11	1:B:376:MET:CE	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:O	1:B:324:LYS:HG3	2.04	0.57
1:A:351:GLN:HB2	4:A:1210:HOH:O	2.03	0.57
1:A:276:THR:HB	1:A:337:VAL:HG13	1.87	0.57
1:B:271:ARG:HD3	1:B:343:THR:OG1	2.04	0.57
1:A:188:MET:HE1	1:A:193:TYR:HD1	1.70	0.57
1:A:446:ARG:CG	1:A:449:LYS:HE3	2.35	0.57
1:A:446:ARG:HA	1:A:449:LYS:HG2	1.88	0.56
1:A:306:ILE:O	1:A:309:LEU:HB3	2.06	0.56
1:A:267:GLU:HG3	1:A:267:GLU:O	2.06	0.55
1:B:3:THR:CG2	1:B:93:ARG:H	2.18	0.55
1:A:236:ALA:HB1	1:A:446:ARG:NH2	2.16	0.55
1:B:110:PHE:CD1	1:B:134:MET:HE2	2.40	0.55
1:B:176:GLU:CB	1:B:225:ASP:HB2	2.34	0.55
1:B:248:GLU:HG3	4:B:1140:HOH:O	2.07	0.55
1:A:258:GLU:HB2	1:A:273:ILE:HD12	1.89	0.55
1:B:373:VAL:O	1:B:377:GLU:HG3	2.07	0.55
1:A:274:LYS:HG3	1:A:306:ILE:HG13	1.88	0.55
1:A:453:LYS:HE3	4:A:1241:HOH:O	2.06	0.55
1:A:396:TYR:C	1:A:397:LEU:HD12	2.32	0.54
1:A:232:GLN:HG2	4:A:1192:HOH:O	2.08	0.54
1:B:103:GLN:O	1:B:157:HIS:HE1	1.91	0.54
1:B:299:ASP:CA	1:B:302:GLU:HB2	2.37	0.54
1:B:269:GLN:CD	1:B:343:THR:HG21	2.32	0.54
1:A:217:ARG:HG2	4:A:1044:HOH:O	2.08	0.54
1:A:446:ARG:HA	1:A:449:LYS:CD	2.37	0.54
1:A:311:ARG:O	1:A:314:ILE:HD13	2.08	0.54
1:A:33:LEU:O	1:A:243:ALA:HA	2.08	0.53
1:B:23:SER:O	1:B:26:SER:HB3	2.08	0.53
1:B:308:ASP:HA	1:B:311:ARG:CZ	2.38	0.53
1:B:35:HIS:CD2	1:B:37:GLY:H	2.22	0.53
1:A:35:HIS:HD2	1:A:37:GLY:N	2.05	0.53
1:A:188:MET:HE1	1:A:193:TYR:CD1	2.44	0.52
1:B:24:ARG:HD2	1:B:170:GLN:HE21	1.73	0.52
1:B:179:THR:HG22	1:B:223:SER:OG	2.09	0.52
1:A:211:GLN:O	1:A:369:GLY:O	2.27	0.52
1:B:24:ARG:CB	1:B:170:GLN:HG3	2.40	0.52
1:B:306:ILE:O	1:B:309:LEU:HB3	2.10	0.52
1:A:65:VAL:HG22	1:A:74:THR:HG22	1.91	0.52
1:A:295:ASN:C	1:A:300:ARG:HD3	2.34	0.52
1:A:325:VAL:O	1:A:325:VAL:HG12	2.09	0.52
1:B:388:ASN:ND2	1:B:389:ALA:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ASP:O	1:B:303:ASN:OD1	2.29	0.51
1:A:192:GLN:O	1:A:196:LYS:HG3	2.10	0.51
1:B:14:ARG:HD3	1:B:16:ASP:OD1	2.10	0.51
1:B:169:SER:O	1:B:170:GLN:O	2.28	0.51
1:A:188:MET:CE	1:A:216:GLN:HB3	2.40	0.51
1:A:329:PHE:HA	1:A:340:LEU:HD11	1.91	0.51
1:A:369:GLY:O	1:A:375:ALA:HB2	2.09	0.51
1:B:35:HIS:HD2	1:B:37:GLY:N	2.06	0.51
1:B:65:VAL:HG22	1:B:74:THR:HG22	1.92	0.51
1:A:446:ARG:CB	1:A:449:LYS:HE3	2.40	0.51
1:A:345:THR:HG22	4:A:1164:HOH:O	2.11	0.50
1:B:35:HIS:CD2	1:B:234:ASN:HD21	2.29	0.50
1:A:367:ILE:HD13	1:A:391:CYS:HB3	1.93	0.50
1:A:449:LYS:HG3	1:A:450:GLN:N	2.26	0.50
1:B:45:ARG:HH21	1:B:149:ARG:HG3	1.76	0.50
1:B:326:PRO:HG3	1:B:343:THR:H	1.76	0.50
1:A:300:ARG:HG3	1:A:300:ARG:O	2.11	0.50
1:B:311:ARG:HB2	1:B:311:ARG:NH1	2.22	0.50
1:B:343:THR:HG22	1:B:345:THR:HG23	1.92	0.50
1:A:190:ARG:HE	1:A:434:GLU:CD	2.19	0.50
1:A:295:ASN:HA	1:A:300:ARG:HD3	1.93	0.50
1:B:190:ARG:HG2	1:B:437:TYR:CE2	2.47	0.50
1:B:343:THR:HG23	1:B:344:ILE:O	2.12	0.50
1:B:190:ARG:NH1	1:B:433:GLU:OE2	2.46	0.49
1:B:306:ILE:HD12	1:B:307:VAL:N	2.28	0.49
1:B:168:GLU:O	1:B:170:GLN:OE1	2.30	0.49
1:A:177:ASP:HA	4:A:1320:HOH:O	2.12	0.49
1:B:206:SER:HB2	1:B:208:ASP:OD1	2.11	0.49
1:B:368:THR:HG22	1:B:369:GLY:O	2.13	0.49
1:B:438:GLN:NE2	1:B:441:PHE:HB2	2.27	0.49
1:A:188:MET:HE3	1:A:193:TYR:HB2	1.95	0.49
1:B:180:LEU:HD23	1:B:222:TYR:HB3	1.94	0.49
1:B:255:LEU:HD22	1:B:255:LEU:N	2.27	0.49
1:B:322:SER:O	1:B:346:ALA:HA	2.13	0.49
1:B:100:LEU:HA	1:B:101:PRO:HD2	1.57	0.49
1:A:188:MET:CE	1:A:193:TYR:HB2	2.43	0.48
1:B:110:PHE:HD1	1:B:134:MET:HE2	1.78	0.48
1:A:35:HIS:CD2	1:A:37:GLY:H	2.25	0.48
1:A:23:SER:HB3	1:A:172:PHE:CE1	2.49	0.48
1:B:312:ASN:O	1:B:316:ARG:HG2	2.14	0.48
1:B:178:PHE:CG	1:B:229:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:VAL:HA	4:B:1288:HOH:O	2.12	0.48
1:A:166:TRP:O	1:A:169:SER:OG	2.29	0.48
1:B:219:HIS:ND1	1:B:418:GLN:OE1	2.47	0.47
1:B:379:ILE:O	1:B:383:GLU:HB2	2.15	0.47
1:A:9:ILE:HD12	1:A:164:ARG:HD3	1.96	0.47
1:A:185:GLN:HB3	1:A:219:HIS:CD2	2.50	0.47
1:B:92:ILE:HG22	1:B:94:PRO:HD3	1.96	0.47
1:B:208:ASP:HB3	1:B:374:ARG:HE	1.77	0.47
1:A:424:GLY:H	3:A:1701:FMT:C	2.26	0.47
1:A:160:VAL:O	1:A:160:VAL:HG22	2.14	0.47
1:B:271:ARG:HG2	1:B:343:THR:OG1	2.15	0.47
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.81	0.47
1:A:52:GLU:HG3	1:A:166:TRP:CZ2	2.50	0.47
1:A:276:THR:HB	1:A:337:VAL:CG1	2.44	0.47
1:B:24:ARG:HB2	1:B:170:GLN:HG3	1.96	0.47
1:A:412:LEU:HD23	1:A:421:CYS:HB2	1.97	0.46
1:B:447:ILE:HD12	4:B:1288:HOH:O	2.15	0.46
1:A:41:HIS:CG	1:A:42:PRO:HD2	2.50	0.46
1:A:270:THR:HG23	1:A:270:THR:O	2.15	0.46
1:A:298:LYS:HD2	1:A:298:LYS:O	2.16	0.46
1:B:271:ARG:NH2	1:B:342:SER:OG	2.49	0.46
1:B:343:THR:HG22	1:B:343:THR:O	2.16	0.46
1:A:198:ARG:HH11	1:A:198:ARG:HD3	1.45	0.45
1:B:80:LEU:HD12	1:B:118:PHE:CZ	2.52	0.45
1:A:17:ALA:HA	1:A:20:PHE:HB3	1.97	0.45
1:B:77:ASP:OD1	1:B:78:ASP:N	2.49	0.45
1:B:134:MET:HG2	1:B:136:VAL:HG23	1.96	0.45
1:A:208:ASP:HB3	1:A:374:ARG:NE	2.27	0.45
1:B:310:MET:O	1:B:314:ILE:HG12	2.16	0.45
1:B:192:GLN:O	1:B:196:LYS:HG3	2.16	0.45
1:B:298:LYS:HG3	1:B:299:ASP:OD1	2.16	0.45
1:B:195:GLU:O	1:B:199:GLN:N	2.48	0.45
1:A:299:ASP:O	1:A:302:GLU:N	2.49	0.45
1:B:1:MET:N	1:B:94:PRO:O	2.49	0.45
1:B:190:ARG:HG2	1:B:437:TYR:CZ	2.52	0.45
1:A:9:ILE:CD1	1:A:164:ARG:HD3	2.47	0.44
1:A:332:GLU:HA	1:A:333:PRO:HD3	1.53	0.44
1:B:300:ARG:HA	1:B:303:ASN:ND2	2.23	0.44
1:A:96:HIS:NE2	1:A:265:ASN:HB2	2.32	0.44
1:A:24:ARG:H	1:A:24:ARG:HG2	1.52	0.44
1:B:303:ASN:O	1:B:306:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD13	1:A:12:LEU:HA	1.62	0.44
1:A:370:ALA:HA	1:A:371:PRO:C	2.42	0.44
1:A:55:CYS:HB3	1:A:138:ILE:HB	1.98	0.44
1:B:176:GLU:O	1:B:228:GLN:HG3	2.18	0.44
1:B:209:CYS:HA	1:B:371:PRO:HD2	2.00	0.44
1:B:438:GLN:NE2	1:B:438:GLN:HA	2.33	0.44
1:B:446:ARG:HA	1:B:449:LYS:HB2	2.00	0.44
1:B:449:LYS:HA	1:B:449:LYS:HD3	1.83	0.44
1:A:97:ASN:OD1	1:A:99:ASP:N	2.46	0.43
1:A:195:GLU:HG2	1:A:199:GLN:HE21	1.83	0.43
1:B:159:ASP:OD1	1:B:161:ASN:N	2.51	0.43
1:A:446:ARG:CA	1:A:449:LYS:HG2	2.48	0.43
1:B:178:PHE:CE2	1:B:451:LEU:HG	2.53	0.43
1:B:186:SER:OG	1:B:187:ASN:N	2.52	0.43
1:B:444:VAL:O	1:B:448:LEU:HG	2.19	0.43
1:A:397:LEU:HD12	1:A:397:LEU:N	2.33	0.43
1:B:190:ARG:HH22	1:B:433:GLU:HG2	1.83	0.43
1:B:449:LYS:HZ2	1:B:449:LYS:HG2	1.64	0.43
1:A:394:ILE:HD13	1:A:394:ILE:HG21	1.76	0.42
1:A:446:ARG:HA	1:A:449:LYS:HD3	2.01	0.42
1:B:265:ASN:O	1:B:266:SER:HB2	2.18	0.42
1:A:390:TRP:CD2	1:A:422:SER:HB2	2.54	0.42
1:B:2:LYS:HB2	1:B:2:LYS:HE2	1.38	0.42
1:B:171:GLN:CA	1:B:171:GLN:HE21	2.33	0.42
1:B:261:ILE:HD13	1:B:261:ILE:HG21	1.61	0.42
1:A:84:GLN:NE2	4:A:1080:HOH:O	2.50	0.42
1:A:149:ARG:NH2	4:A:1261:HOH:O	2.51	0.42
1:A:424:GLY:N	3:A:1701:FMT:H	2.31	0.42
1:B:190:ARG:HH12	1:B:433:GLU:CG	2.32	0.42
1:A:323:VAL:HA	1:A:345:THR:O	2.19	0.42
1:B:271:ARG:HD3	1:B:343:THR:HA	2.02	0.42
1:B:310:MET:O	1:B:313:ASP:HB2	2.20	0.42
1:A:188:MET:HE3	1:A:188:MET:HB3	1.85	0.42
1:A:276:THR:O	1:A:277:LEU:HD13	2.19	0.41
1:A:23:SER:O	1:A:172:PHE:HD1	2.03	0.41
1:B:196:LYS:O	1:B:200:VAL:N	2.50	0.41
1:A:61:GLY:O	1:A:117:ARG:HD3	2.20	0.41
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.85	0.41
1:B:188:MET:CG	1:B:216:GLN:HG2	2.51	0.41
1:A:116:ARG:HH11	1:A:116:ARG:HD3	1.59	0.41
1:A:274:LYS:HG3	1:A:306:ILE:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HG21	1:B:129:ILE:HD13	1.82	0.41
1:A:4:LEU:H	1:A:4:LEU:HG	1.30	0.41
1:A:295:ASN:CA	1:A:300:ARG:HD3	2.51	0.41
1:B:193:TYR:CE2	1:B:437:TYR:HB2	2.55	0.41
1:A:279:ARG:HD2	1:A:279:ARG:HA	1.67	0.41
1:A:190:ARG:NH2	1:A:434:GLU:OE1	2.50	0.41
1:B:297:ALA:HB3	1:B:300:ARG:HD3	2.02	0.41
1:A:141:TRP:CE2	1:A:163:ARG:HD2	2.56	0.41
1:A:259:ARG:HH11	1:A:269:GLN:NE2	2.19	0.41
1:A:260:PHE:O	1:A:270:THR:HA	2.21	0.41
1:A:402:ASN:HB3	4:A:1237:HOH:O	2.20	0.41
1:B:110:PHE:CE1	1:B:134:MET:HE2	2.56	0.41
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.93	0.41
1:A:255:LEU:N	1:A:255:LEU:HD22	2.36	0.40
1:A:329:PHE:CA	1:A:340:LEU:HD11	2.51	0.40
1:B:188:MET:HG3	1:B:216:GLN:HG2	2.03	0.40
1:B:381:GLU:HG2	1:B:382:LEU:CD2	2.45	0.40
1:A:274:LYS:HD3	1:A:274:LYS:HA	1.38	0.40
1:B:47:ASP:OD2	1:B:147:HIS:NE2	2.49	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	433/453 (96%)	401 (93%)	25 (6%)	7 (2%)	7	3
1	B	408/453 (90%)	372 (91%)	27 (7%)	9 (2%)	5	2
All	All	841/906 (93%)	773 (92%)	52 (6%)	16 (2%)	6	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	301	ALA
1	B	170	GLN
1	B	173	SER
1	B	298	LYS
1	B	429	ALA
1	A	296	SER
1	B	343	THR
1	A	69	SER
1	B	450	GLN
1	A	176	GLU
1	A	158	ASN
1	A	370	ALA
1	B	449	LYS
1	B	207	GLY
1	B	326	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/390 (96%)	334 (89%)	41 (11%)	6	3
1	B	355/390 (91%)	293 (82%)	62 (18%)	2	1
All	All	730/780 (94%)	627 (86%)	103 (14%)	3	2

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	LEU
1	A	12	LEU
1	A	24	ARG
1	A	27	HIS
1	A	29	PRO
1	A	52	GLU
1	A	62	LYS

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Mol	Chain	Res	Type
1	A	71	LYS
1	A	89	ARG
1	A	93	ARG
1	A	95	THR
1	A	136	VAL
1	A	143	LEU
1	A	148	GLN
1	A	151	THR
1	A	160	VAL
1	A	167	LEU
1	A	168	GLU
1	A	180	LEU
1	A	205	HIS
1	A	209	CYS
1	A	219	HIS
1	A	232	GLN
1	A	238	ARG
1	A	257	PRO
1	A	267	GLU
1	A	274	LYS
1	A	277	LEU
1	A	296	SER
1	A	298	LYS
1	A	300	ARG
1	A	304	LEU
1	A	314	ILE
1	A	316	ARG
1	A	317	VAL
1	A	331	VAL
1	A	335	PRO
1	A	337	VAL
1	A	350	GLU
1	A	453	LYS
1	B	1	MET
1	B	2	LYS
1	B	3	THR
1	B	10	THR
1	B	12	LEU
1	B	15	GLN
1	B	24	ARG
1	B	26	SER
1	B	43	TYR

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Mol	Chain	Res	Type
1	B	62	LYS
1	B	70	GLU
1	B	71	LYS
1	B	75	THR
1	B	83	LEU
1	B	91	ASP
1	B	95	THR
1	B	100	LEU
1	B	158	ASN
1	B	159	ASP
1	B	167	LEU
1	B	169	SER
1	B	171	GLN
1	B	173	SER
1	B	175	GLN
1	B	176	GLU
1	B	190	ARG
1	B	200	VAL
1	B	204	LEU
1	B	206	SER
1	B	219	HIS
1	B	232	GLN
1	B	235	GLN
1	B	238	ARG
1	B	248	GLU
1	B	267	GLU
1	B	271	ARG
1	B	298	LYS
1	B	302	GLU
1	B	303	ASN
1	B	305	MET
1	B	311	ARG
1	B	314	ILE
1	B	317	VAL
1	B	319	VAL
1	B	324	LYS
1	B	326	PRO
1	B	343	THR
1	B	345	THR
1	B	350	GLU
1	B	368	THR
1	B	415	ILE

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Mol	Chain	Res	Type
1	B	418	GLN
1	B	431	SER
1	B	438	GLN
1	B	439	GLU
1	B	443	LYS
1	B	445	ASN
1	B	446	ARG
1	B	449	LYS
1	B	450	GLN
1	B	451	LEU
1	B	453	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	35	HIS
1	A	84	GLN
1	A	85	GLN
1	A	158	ASN
1	A	199	GLN
1	A	201	GLN
1	A	211	GLN
1	A	219	HIS
1	A	269	GLN
1	A	339	HIS
1	A	416	ASN
1	A	450	GLN
1	B	35	HIS
1	B	81	GLN
1	B	157	HIS
1	B	170	GLN
1	B	171	GLN
1	B	175	GLN
1	B	228	GLN
1	B	232	GLN
1	B	235	GLN
1	B	265	ASN
1	B	303	ASN
1	B	353	HIS
1	B	388	ASN
1	B	438	GLN

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Mol	Chain	Res	Type
1	B	445	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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$
2	TRP	B	602	-	15,16,16	1.39	2 (13%)	18,22,22	2.79	9 (50%)
2	TRP	A	601	-	15,16,16	1.32	1 (6%)	18,22,22	2.40	10 (55%)
3	FMT	A	1701	-	2,2,2	6.18	2 (100%)	1,1,1	1.12	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
2	TRP	B	602	-	-	0/8/8/8	0/2/2/2
2	TRP	A	601	-	-	0/8/8/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1701	FMT	O2-C	6.38	1.61	1.28
3	A	1701	FMT	O1-C	5.97	1.55	1.22
2	A	601	TRP	CH2-CZ3	3.44	1.45	1.38
2	B	602	TRP	CD1-NE1	2.38	1.41	1.37
2	B	602	TRP	CB-CG	2.26	1.54	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	TRP	CZ3-CH2-CZ2	5.76	127.35	120.24
2	B	602	TRP	CZ3-CE3-CD2	-4.59	111.50	119.80
2	B	602	TRP	CH2-CZ2-CE2	-4.49	109.56	118.69
2	A	601	TRP	OXT-C-O	-4.21	114.54	124.08
2	B	602	TRP	CE3-CD2-CE2	3.64	122.61	118.84
2	A	601	TRP	CE3-CD2-CE2	-3.64	115.07	118.84
2	B	602	TRP	CZ2-CE2-CD2	3.55	125.62	122.19
2	B	602	TRP	CZ2-CE2-NE1	-3.28	125.48	130.74
2	A	601	TRP	CH2-CZ2-CE2	3.15	125.09	118.69
2	A	601	TRP	CE3-CD2-CG	3.01	138.34	133.85
2	A	601	TRP	CZ3-CE3-CD2	3.01	125.23	119.80
2	A	601	TRP	CE2-NE1-CD1	2.91	111.66	109.08
2	A	601	TRP	CZ3-CH2-CZ2	-2.89	116.68	120.24
2	A	601	TRP	CG-CD1-NE1	-2.86	107.16	110.31
2	B	602	TRP	CE3-CD2-CG	-2.65	129.90	133.85
2	B	602	TRP	CH2-CZ3-CE3	2.53	123.36	120.24
2	B	602	TRP	CE2-NE1-CD1	-2.48	106.87	109.08
2	A	601	TRP	CA-CB-CG	-2.32	109.09	113.49
2	A	601	TRP	CH2-CZ3-CE3	-2.08	117.67	120.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	TRP	1	0
3	A	1701	FMT	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/453 (96%)	-0.12	15 (3%) 48 47	9, 23, 51, 73	0
1	B	414/453 (91%)	0.20	31 (7%) 20 19	11, 27, 66, 144	0
All	All	851/906 (93%)	0.04	46 (5%) 31 30	9, 24, 60, 144	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	PHE	5.4
1	B	299	ASP	4.7
1	B	176	GLU	4.6
1	B	1	MET	3.9
1	B	173	SER	3.8
1	B	453	LYS	3.7
1	B	312	ASN	3.7
1	A	207	GLY	3.6
1	A	3	THR	3.5
1	B	343	THR	3.5
1	B	175	GLN	3.4
1	A	205	HIS	3.4
1	B	170	GLN	3.3
1	B	174	PRO	3.3
1	B	43	TYR	3.3
1	B	297	ALA	3.2
1	A	453	LYS	3.2
1	B	320	ALA	3.2
1	A	294	ALA	3.1
1	B	305	MET	3.0
1	B	303	ASN	2.8
1	A	175	GLN	2.8
1	A	300	ARG	2.7
1	B	321	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	298	LYS	2.7
1	A	42	PRO	2.6
1	A	210	TYR	2.5
1	B	37	GLY	2.4
1	A	176	GLU	2.4
1	B	171	GLN	2.4
1	B	327	GLU	2.3
1	B	311	ARG	2.3
1	B	69	SER	2.3
1	B	309	LEU	2.3
1	B	41	HIS	2.3
1	A	297	ALA	2.3
1	A	169	SER	2.2
1	A	208	ASP	2.2
1	B	326	PRO	2.1
1	A	267	GLU	2.1
1	B	2	LYS	2.1
1	B	12	LEU	2.1
1	B	439	GLU	2.1
1	B	205	HIS	2.0
1	B	308	ASP	2.0
1	A	321	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMT	A	1701	3/3	0.82	0.10	22,22,25,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	B	602	15/15	0.93	0.07	11,17,22,22	0
2	TRP	A	601	15/15	0.94	0.06	8,15,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.