



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 3PGA / pdb_00003pga
Title : STRUCTURAL CHARACTERIZATION OF PSEUDOMONAS 7A GLUTAMINASE-ASPARAGINASE
Authors : Lubkowski, J.; Wlodawer, A.; Ammon, H.L.; Copeland, T.D.; Swain, A.L.
Deposited on : 1994-07-19
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
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

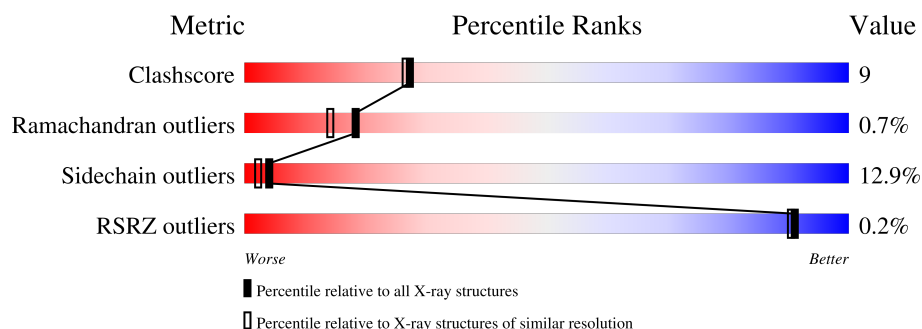
1 Overall quality at a glance

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))
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	1	337	36% 46% 12% ..
1	2	337	43% 39% 14% ..
1	3	337	45% 37% 13% ..
1	4	337	41% 42% 13% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10854 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 GLUTAMINASE-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	330	Total	C	N	O	S	253	20	0
			2611	1627	459	518	7			
1	2	330	Total	C	N	O	S	126	20	0
			2611	1627	459	518	7			
1	3	329	Total	C	N	O	S	253	20	0
			2607	1625	458	517	7			
1	4	329	Total	C	N	O	S	253	20	0
			2607	1625	458	517	7			

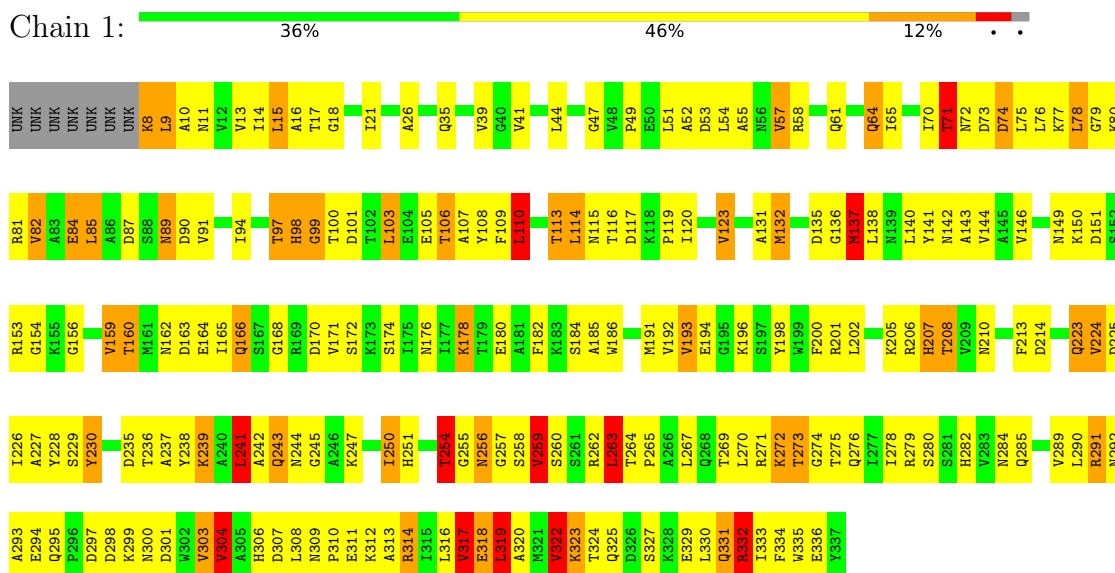
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	113	Total	O	0	0
			113	113		
2	2	87	Total	O	0	0
			87	87		
2	3	112	Total	O	0	0
			112	112		
2	4	106	Total	O	0	0
			106	106		

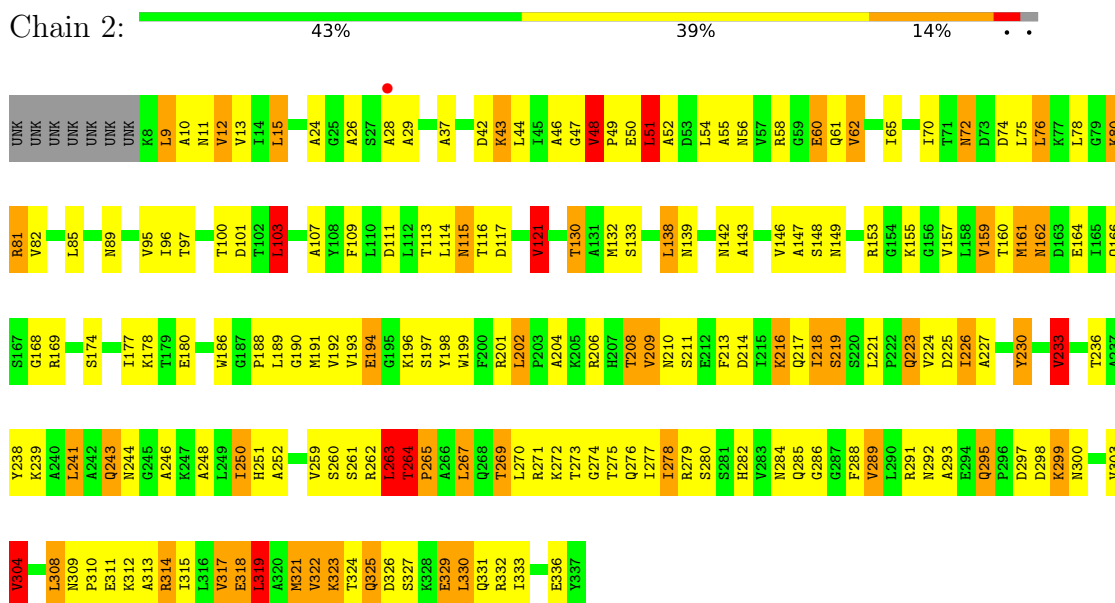
3 Residue-property plots

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.

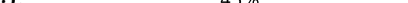
• Molecule 1: GLUTAMINASE-ASPARAGINASE

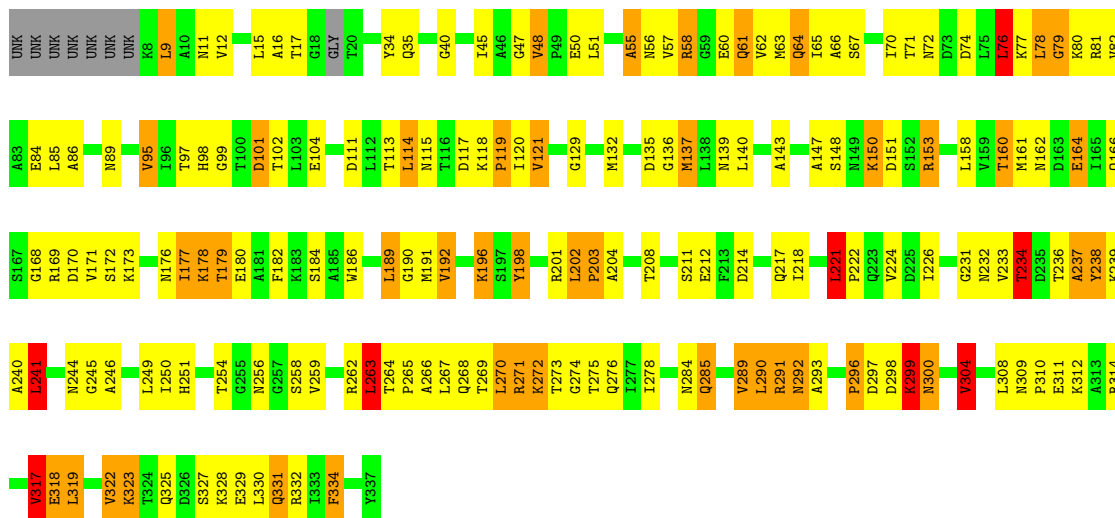


• Molecule 1: GLUTAMINASE-ASPARAGINASE

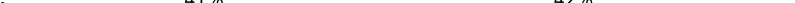


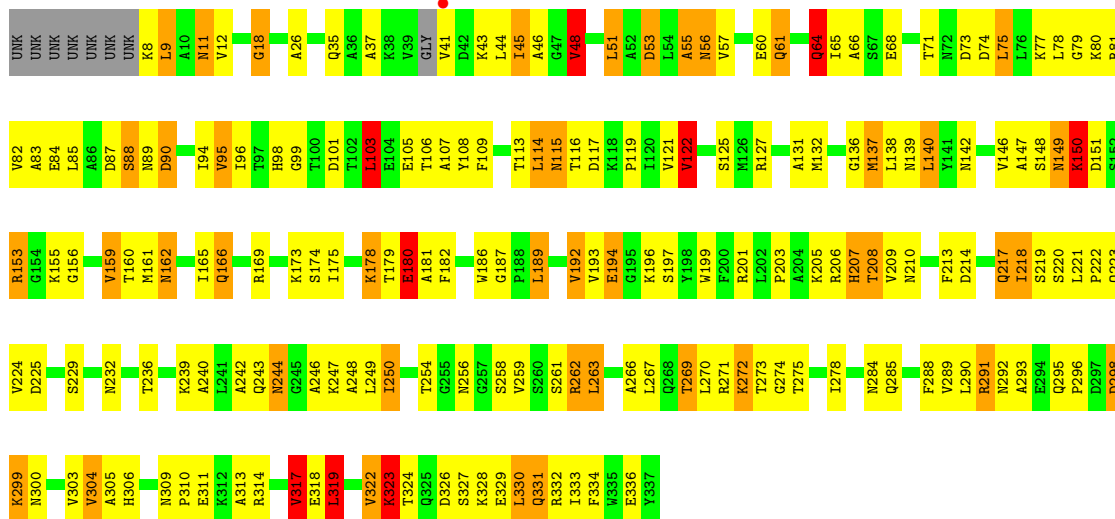
- Molecule 1: GLUTAMINASE-ASPARAGINASE

Chain 3:  45% 37% 13% ..



- Molecule 1: GLUTAMINASE-ASPARAGINASE

Chain 4:  41% 42% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.26Å 130.75Å 85.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (10.00-2.00) 46.7 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.165 , (Not available) 0.140 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.2	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10854	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 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

5.1 Standard geometry

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	1	1.42	7/2391 (0.3%)	3.02	318/3238 (9.8%)
1	2	1.36	5/2391 (0.2%)	2.95	271/3238 (8.4%)
1	3	1.40	5/2387 (0.2%)	2.86	254/3233 (7.9%)
1	4	1.39	5/2387 (0.2%)	3.01	298/3233 (9.2%)
All	All	1.39	22/9556 (0.2%)	2.96	1141/12942 (8.8%)

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	1	0	3
1	2	0	1
1	3	0	3
1	4	0	3
All	All	0	10

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	226	ILE	CA-CB	7.96	1.64	1.54
1	4	269	THR	CB-OG1	6.39	1.53	1.43
1	1	202	LEU	N-CA	6.30	1.50	1.45
1	1	276	GLN	N-CA	5.92	1.53	1.46
1	3	113	THR	CA-CB	5.87	1.62	1.54
1	2	269	THR	CB-OG1	5.82	1.53	1.43
1	1	18	GLY	C-O	5.81	1.28	1.24
1	2	188	PRO	CA-C	5.75	1.59	1.52
1	4	66	ALA	N-CA	5.63	1.53	1.46
1	3	273	THR	CB-OG1	5.58	1.52	1.43
1	1	317	VAL	C-N	-5.48	1.26	1.33
1	1	250	ILE	CB-CG1	5.47	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	273	THR	CB-OG1	5.40	1.52	1.43
1	4	306	HIS	C-O	5.19	1.29	1.24
1	2	233	VAL	CA-C	5.11	1.59	1.52
1	3	114	LEU	CA-CB	5.10	1.59	1.53
1	4	113	THR	CA-CB	5.08	1.61	1.53
1	2	208	THR	C-N	-5.07	1.27	1.34
1	1	334	PHE	N-CA	5.01	1.52	1.46
1	3	237	ALA	N-CA	5.01	1.52	1.46
1	2	226	ILE	CA-CB	5.00	1.60	1.54
1	3	153	ARG	NE-CZ	5.00	1.38	1.33

All (1141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	81	ARG	CD-NE-CZ	19.37	151.52	124.40
1	4	115	ASN	CA-CB-CG	17.94	130.54	112.60
1	2	72	ASN	CB-CA-C	17.64	146.85	109.99
1	4	244	ASN	OD1-CG-ND2	16.06	138.66	122.60
1	1	262	ARG	NE-CZ-NH2	-15.37	105.37	119.20
1	3	244	ASN	OD1-CG-ND2	15.10	137.70	122.60
1	2	72	ASN	CB-CG-ND2	15.00	138.91	116.40
1	4	115	ASN	OD1-CG-ND2	-14.55	108.05	122.60
1	2	72	ASN	CA-CB-CG	14.47	127.07	112.60
1	2	115	ASN	CA-CB-CG	14.03	126.62	112.60
1	1	176	ASN	OD1-CG-ND2	13.88	136.48	122.60
1	3	114	LEU	CB-CA-C	13.85	134.58	111.31
1	3	323	LYS	CA-CB-CG	13.82	141.75	114.10
1	1	254	THR	N-CA-CB	-13.60	89.77	110.45
1	3	115	ASN	CA-CB-CG	13.40	126.00	112.60
1	4	332	ARG	NE-CZ-NH2	-13.38	107.16	119.20
1	1	293	ALA	CA-C-O	-13.21	107.01	120.89
1	2	300	ASN	CA-CB-CG	13.21	125.81	112.60
1	3	89	ASN	CA-CB-CG	-12.86	99.74	112.60
1	2	314	ARG	NE-CZ-NH2	12.83	130.74	119.20
1	1	262	ARG	CA-CB-CG	12.82	139.74	114.10
1	2	325	GLN	CB-CG-CD	12.75	134.27	112.60
1	1	263	LEU	CD1-CG-CD2	12.74	138.83	110.80
1	4	122	VAL	CB-CA-C	12.72	129.78	110.83
1	1	272	LYS	CA-CB-CG	12.66	139.42	114.10
1	4	150	LYS	CB-CG-CD	12.51	140.07	111.30
1	2	96	ILE	CA-C-O	-12.51	107.39	120.39
1	1	53	ASP	CA-CB-CG	12.46	125.06	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	115	ASN	CA-CB-CG	12.17	124.77	112.60
1	1	58	ARG	CD-NE-CZ	12.03	141.24	124.40
1	2	114	LEU	CB-CA-C	12.02	131.88	111.68
1	4	271	ARG	NE-CZ-NH2	12.00	130.00	119.20
1	3	318	GLU	CA-C-O	12.00	133.27	120.55
1	1	114	LEU	CB-CA-C	11.86	131.23	111.31
1	1	99	GLY	CA-C-O	-11.70	111.11	121.41
1	4	81	ARG	CD-NE-CZ	11.63	140.69	124.40
1	4	263	LEU	N-CA-CB	-11.62	95.44	110.90
1	3	234	THR	CA-CB-CG2	11.61	130.23	110.50
1	4	244	ASN	CA-CB-CG	-11.42	101.18	112.60
1	1	273	THR	CB-CA-C	11.41	130.54	110.81
1	2	166	GLN	OE1-CD-NE2	-11.40	111.20	122.60
1	4	53	ASP	CA-CB-CG	11.34	123.94	112.60
1	2	233	VAL	CB-CA-C	-11.24	95.77	111.28
1	3	120	ILE	CA-C-O	-11.19	108.75	120.39
1	1	98	HIS	CA-CB-CG	11.15	124.95	113.80
1	1	317	VAL	CA-C-O	-11.01	109.50	121.17
1	3	115	ASN	OD1-CG-ND2	-10.96	111.64	122.60
1	4	9	LEU	CB-CA-C	10.82	128.01	109.51
1	3	162	ASN	OD1-CG-ND2	10.79	133.40	122.60
1	1	250	ILE	CB-CG1-CD1	-10.79	91.15	113.80
1	4	114	LEU	CB-CA-C	10.74	129.62	111.68
1	4	114	LEU	CD1-CG-CD2	-10.68	87.31	110.80
1	3	317	VAL	CA-C-O	-10.61	108.79	120.25
1	4	221	LEU	N-CA-CB	-10.60	91.47	110.23
1	3	263	LEU	CD1-CG-CD2	10.59	134.09	110.80
1	1	193	VAL	CB-CA-C	10.49	123.21	110.73
1	4	179	THR	CA-CB-OG1	-10.44	93.94	109.60
1	3	114	LEU	CB-CG-CD1	10.38	141.84	110.70
1	1	263	LEU	N-CA-C	10.34	127.21	113.97
1	1	18	GLY	N-CA-C	-10.32	101.14	111.56
1	3	64	GLN	OE1-CD-NE2	-10.31	112.29	122.60
1	4	299	LYS	CB-CG-CD	10.29	134.98	111.30
1	1	244	ASN	CB-CG-ND2	-10.24	101.04	116.40
1	1	327	SER	CA-CB-OG	-10.21	90.69	111.10
1	4	262	ARG	CA-CB-CG	10.14	134.39	114.10
1	2	13	VAL	CA-C-O	-10.08	109.79	120.48
1	4	147	ALA	CA-C-N	10.07	138.77	121.14
1	4	147	ALA	C-N-CA	10.07	138.77	121.14
1	3	234	THR	N-CA-CB	-10.06	95.96	111.05
1	2	60	GLU	N-CA-CB	10.04	129.31	111.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	292	ASN	OD1-CG-ND2	-9.98	112.62	122.60
1	1	256	ASN	OD1-CG-ND2	-9.93	112.67	122.60
1	1	254	THR	CA-CB-CG2	9.93	127.38	110.50
1	1	263	LEU	N-CA-CB	-9.92	96.88	110.67
1	2	241	LEU	CA-C-O	-9.91	110.49	120.70
1	1	325	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	1	273	THR	CA-CB-OG1	9.88	124.41	109.60
1	1	273	THR	OG1-CB-CG2	-9.86	89.59	109.30
1	1	149	ASN	CA-CB-CG	9.85	122.45	112.60
1	3	309	ASN	OD1-CG-ND2	-9.81	112.79	122.60
1	1	114	LEU	CD1-CG-CD2	-9.78	89.29	110.80
1	3	285	GLN	OE1-CD-NE2	9.76	132.36	122.60
1	1	309	ASN	CA-CB-CG	9.74	122.34	112.60
1	2	217	GLN	OE1-CD-NE2	9.72	132.32	122.60
1	1	273	THR	O-C-N	-9.69	109.97	122.37
1	3	98	HIS	CA-CB-CG	9.67	123.47	113.80
1	1	180	GLU	CB-CG-CD	9.65	129.01	112.60
1	4	194	GLU	CA-CB-CG	9.61	133.33	114.10
1	4	162	ASN	CA-CB-CG	9.61	122.21	112.60
1	1	273	THR	CA-C-O	9.61	131.41	119.59
1	4	175	ILE	CA-C-O	-9.58	110.33	120.39
1	4	96	ILE	CA-C-O	-9.57	110.43	120.39
1	2	169	ARG	CD-NE-CZ	9.55	137.78	124.40
1	3	196	LYS	CA-C-O	-9.53	110.61	120.71
1	4	8	LYS	CA-CB-CG	9.53	133.16	114.10
1	1	115	ASN	CB-CG-ND2	9.51	130.67	116.40
1	4	262	ARG	NE-CZ-NH2	-9.50	110.65	119.20
1	3	64	GLN	CB-CA-C	9.48	124.70	111.23
1	1	151	ASP	CA-CB-CG	9.48	122.08	112.60
1	3	101	ASP	O-C-N	9.48	132.17	122.12
1	2	295	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	4	285	GLN	CB-CA-C	9.43	126.98	110.01
1	3	114	LEU	CD1-CG-CD2	-9.42	90.08	110.80
1	2	149	ASN	CA-CB-CG	9.42	122.02	112.60
1	1	245	GLY	CA-C-O	-9.40	108.42	119.04
1	1	311	GLU	CB-CG-CD	9.39	128.57	112.60
1	1	192	VAL	N-CA-CB	9.39	123.84	111.64
1	1	64	GLN	CB-CG-CD	9.37	128.53	112.60
1	3	319	LEU	N-CA-CB	-9.35	96.32	110.16
1	2	325	GLN	OE1-CD-NE2	-9.35	113.25	122.60
1	3	275	THR	CA-C-O	-9.33	110.00	120.54
1	3	292	ASN	CB-CG-ND2	9.29	130.34	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	332	ARG	O-C-N	9.29	131.63	122.07
1	1	194	GLU	CB-CG-CD	9.26	128.34	112.60
1	1	206	ARG	NE-CZ-NH2	-9.25	110.87	119.20
1	1	84	GLU	CA-CB-CG	9.24	132.58	114.10
1	4	114	LEU	CB-CG-CD2	9.20	138.30	110.70
1	2	271	ARG	CD-NE-CZ	9.15	137.21	124.40
1	4	285	GLN	CA-CB-CG	9.07	132.23	114.10
1	2	284	ASN	N-CA-C	9.04	124.03	112.92
1	3	323	LYS	CG-CD-CE	9.02	132.04	111.30
1	2	262	ARG	NE-CZ-NH2	-9.01	111.09	119.20
1	3	289	VAL	CB-CA-C	9.01	122.08	110.91
1	4	65	ILE	O-C-N	8.99	132.89	123.00
1	3	135	ASP	CA-CB-CG	8.97	121.57	112.60
1	2	243	GLN	OE1-CD-NE2	8.94	131.53	122.60
1	3	232	ASN	OD1-CG-ND2	-8.94	113.67	122.60
1	3	192	VAL	CB-CA-C	8.92	122.47	110.42
1	1	180	GLU	CA-CB-CG	8.89	131.89	114.10
1	4	174	SER	O-C-N	8.88	133.23	122.48
1	4	221	LEU	CB-CA-C	8.88	121.41	109.42
1	2	244	ASN	CA-CB-CG	-8.85	103.75	112.60
1	4	74	ASP	CA-CB-CG	8.85	121.45	112.60
1	1	198	TYR	CA-C-O	-8.84	110.87	120.24
1	2	81	ARG	CB-CG-CD	8.82	131.59	111.30
1	3	66	ALA	N-CA-C	-8.81	94.15	108.52
1	2	192	VAL	CB-CA-C	8.81	122.31	110.42
1	1	304	VAL	CB-CA-C	8.77	123.35	110.98
1	1	71	THR	N-CA-CB	-8.76	97.01	111.20
1	4	319	LEU	CD1-CG-CD2	8.75	130.05	110.80
1	4	181	ALA	O-C-N	8.68	131.32	122.12
1	1	65	ILE	CA-C-O	8.66	130.21	121.63
1	1	58	ARG	CA-CB-CG	8.66	131.41	114.10
1	2	230	TYR	CA-C-O	-8.64	111.84	121.25
1	2	139	ASN	OD1-CG-ND2	-8.63	113.97	122.60
1	4	159	VAL	CA-C-O	-8.61	111.34	120.39
1	3	169	ARG	NE-CZ-NH2	8.60	126.94	119.20
1	2	48	VAL	CB-CA-C	8.58	126.98	111.36
1	3	114	LEU	O-C-N	-8.56	112.34	122.87
1	4	136	GLY	N-CA-C	8.55	123.00	112.73
1	2	121	VAL	CA-CB-CG1	8.55	124.93	110.40
1	2	115	ASN	O-C-N	-8.54	110.33	122.29
1	4	271	ARG	NH1-CZ-NH2	-8.52	108.22	119.30
1	2	206	ARG	NE-CZ-NH1	8.51	130.01	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	89	ASN	CA-CB-CG	8.50	121.10	112.60
1	2	273	THR	CB-CA-C	8.49	125.49	110.81
1	3	81	ARG	NE-CZ-NH2	8.49	126.84	119.20
1	4	64	GLN	OE1-CD-NE2	-8.47	114.13	122.60
1	4	225	ASP	CA-CB-CG	8.46	121.06	112.60
1	3	168	GLY	N-CA-C	-8.43	103.96	114.16
1	1	236	THR	CA-C-O	-8.42	111.81	121.07
1	1	123	VAL	CB-CA-C	-8.41	95.66	110.71
1	2	263	LEU	N-CA-CB	-8.40	99.72	110.90
1	1	71	THR	CA-CB-CG2	8.39	124.77	110.50
1	4	319	LEU	CA-C-O	-8.39	111.57	120.55
1	1	304	VAL	N-CA-CB	-8.38	97.44	110.86
1	3	271	ARG	CD-NE-CZ	8.37	136.12	124.40
1	2	325	GLN	CA-C-O	8.37	128.46	119.34
1	2	209	VAL	N-CA-CB	-8.34	97.44	110.54
1	4	220	SER	CA-CB-OG	-8.34	94.42	111.10
1	2	226	ILE	CA-C-N	8.34	134.75	122.99
1	2	226	ILE	C-N-CA	8.34	134.75	122.99
1	1	244	ASN	CA-C-N	-8.33	110.88	122.63
1	1	244	ASN	C-N-CA	-8.33	110.88	122.63
1	2	323	LYS	CA-C-O	-8.33	110.00	119.41
1	1	262	ARG	NE-CZ-NH1	8.32	129.82	121.50
1	2	251	HIS	CA-C-O	-8.31	111.69	120.58
1	2	322	VAL	N-CA-C	-8.31	100.31	111.44
1	4	207	HIS	CA-C-O	-8.30	112.43	121.31
1	3	50	GLU	CG-CD-OE1	8.29	137.47	118.40
1	3	259	VAL	CA-C-O	-8.29	111.57	120.36
1	3	237	ALA	CA-C-N	8.29	131.59	120.65
1	3	237	ALA	C-N-CA	8.29	131.59	120.65
1	4	210	ASN	CB-CA-C	8.26	124.68	110.72
1	1	284	ASN	N-CA-C	8.25	123.57	113.17
1	3	284	ASN	N-CA-C	8.25	123.57	113.17
1	1	244	ASN	CB-CA-C	8.25	125.05	110.37
1	2	190	GLY	CA-C-O	-8.23	111.86	121.08
1	4	61	GLN	CA-C-O	-8.21	111.79	120.58
1	4	160	THR	CA-CB-OG1	-8.21	97.28	109.60
1	2	318	GLU	CB-CA-C	-8.21	97.68	110.81
1	4	318	GLU	CA-C-O	8.21	129.41	119.97
1	1	114	LEU	CB-CG-CD2	8.20	135.31	110.70
1	3	204	ALA	CA-C-O	-8.20	110.03	119.05
1	3	311	GLU	CG-CD-OE1	8.18	137.20	118.40
1	4	98	HIS	CA-CB-CG	8.17	121.97	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	303	VAL	CA-C-N	8.15	133.62	123.10
1	4	303	VAL	C-N-CA	8.15	133.62	123.10
1	2	162	ASN	CA-CB-CG	8.13	120.73	112.60
1	3	58	ARG	NH1-CZ-NH2	8.13	129.87	119.30
1	1	334	PHE	CA-C-O	8.13	129.38	119.38
1	1	61	GLN	CA-C-O	-8.13	112.09	120.54
1	2	95	VAL	CA-C-O	-8.13	111.86	120.48
1	3	296	PRO	N-CA-CB	-8.12	97.13	102.65
1	4	121	VAL	O-C-N	8.12	132.03	123.26
1	1	194	GLU	CA-CB-CG	8.11	130.32	114.10
1	3	111	ASP	CA-CB-CG	8.10	120.70	112.60
1	2	269	THR	CA-CB-CG2	8.10	124.27	110.50
1	4	95	VAL	CB-CA-C	8.06	122.63	110.62
1	2	295	GLN	CG-CD-NE2	8.06	128.49	116.40
1	2	319	LEU	CD1-CG-CD2	8.05	128.52	110.80
1	2	55	ALA	O-C-N	8.04	131.60	122.99
1	2	314	ARG	CD-NE-CZ	8.04	135.66	124.40
1	1	64	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	2	72	ASN	CB-CG-OD1	-8.00	104.80	120.80
1	1	205	LYS	CA-C-N	7.98	132.15	120.90
1	1	205	LYS	C-N-CA	7.98	132.15	120.90
1	3	147	ALA	CA-C-N	7.98	135.11	121.14
1	3	147	ALA	C-N-CA	7.98	135.11	121.14
1	3	319	LEU	CD1-CG-CD2	7.98	128.35	110.80
1	3	177	ILE	CA-C-O	-7.97	110.81	120.78
1	1	210	ASN	CA-C-O	7.97	129.00	119.59
1	1	262	ARG	CB-CA-C	7.97	125.81	109.95
1	1	289	VAL	CA-C-O	7.96	129.70	120.71
1	4	81	ARG	NE-CZ-NH2	7.95	126.35	119.20
1	2	149	ASN	CB-CA-C	7.94	123.45	109.72
1	4	275	THR	CA-CB-OG1	-7.93	97.70	109.60
1	3	292	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	3	153	ARG	NE-CZ-NH2	-7.93	112.06	119.20
1	3	289	VAL	CA-CB-CG1	7.93	123.88	110.40
1	4	166	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	2	304	VAL	CB-CA-C	7.92	122.15	110.98
1	2	80	LYS	CB-CG-CD	7.92	129.51	111.30
1	3	153	ARG	CA-C-O	-7.92	113.16	121.55
1	4	236	THR	CA-C-O	-7.89	112.45	120.90
1	3	147	ALA	CA-C-O	-7.88	112.19	120.55
1	4	262	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	2	304	VAL	N-CA-CB	-7.87	98.27	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	310	PRO	O-C-N	-7.87	113.68	122.18
1	2	327	SER	O-C-N	7.86	131.42	122.22
1	3	275	THR	O-C-N	7.85	132.16	123.22
1	1	100	THR	N-CA-C	7.84	122.11	112.54
1	1	319	LEU	CA-C-N	7.84	130.78	120.28
1	1	319	LEU	C-N-CA	7.84	130.78	120.28
1	3	218	ILE	CA-C-O	-7.83	112.15	120.53
1	2	269	THR	CA-C-O	-7.83	111.55	120.24
1	2	97	THR	CA-CB-OG1	-7.82	97.87	109.60
1	4	284	ASN	CA-C-O	-7.80	110.23	119.35
1	1	159	VAL	CB-CA-C	7.79	122.16	110.63
1	4	174	SER	CA-C-O	-7.79	110.64	118.97
1	2	318	GLU	N-CA-CB	7.78	121.53	109.94
1	4	83	ALA	CA-C-O	-7.78	112.31	120.55
1	4	213	PHE	CA-C-O	-7.77	112.38	121.16
1	2	114	LEU	CD1-CG-CD2	-7.77	93.71	110.80
1	4	94	ILE	CA-C-N	-7.74	112.38	123.06
1	4	94	ILE	C-N-CA	-7.74	112.38	123.06
1	1	274	GLY	N-CA-C	7.73	126.99	115.08
1	1	196	LYS	N-CA-CB	7.72	123.13	110.69
1	3	332	ARG	CB-CG-CD	7.72	129.06	111.30
1	1	120	ILE	CA-C-O	-7.72	112.36	120.39
1	4	270	LEU	N-CA-C	-7.72	102.95	111.36
1	3	246	ALA	CA-C-O	-7.71	111.94	120.81
1	2	204	ALA	N-CA-C	-7.69	103.72	113.72
1	2	96	ILE	O-C-N	7.69	131.35	123.20
1	2	159	VAL	CB-CA-C	7.69	121.56	110.33
1	3	150	LYS	CB-CG-CD	7.68	128.97	111.30
1	4	77	LYS	CB-CG-CD	7.67	128.94	111.30
1	3	259	VAL	O-C-N	7.65	131.46	123.20
1	3	55	ALA	O-C-N	7.64	130.99	123.04
1	4	150	LYS	CG-CD-CE	7.64	128.88	111.30
1	4	317	VAL	CB-CA-C	-7.63	101.69	112.22
1	2	65	ILE	CA-C-O	7.60	129.16	121.63
1	3	308	LEU	O-C-N	7.58	132.25	122.93
1	2	331	GLN	N-CA-CB	7.57	120.98	110.01
1	4	300	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	4	156	GLY	CA-C-O	-7.56	114.77	122.56
1	1	239	LYS	CB-CA-C	-7.54	98.27	110.79
1	1	280	SER	O-C-N	-7.54	114.54	122.84
1	2	81	ARG	CG-CD-NE	7.54	128.59	112.00
1	2	12	VAL	CB-CA-C	7.53	121.84	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	14	ILE	CA-C-O	-7.53	112.39	120.59
1	3	293	ALA	CA-C-O	-7.52	112.99	120.89
1	3	84	GLU	CA-C-O	-7.52	112.58	120.55
1	4	328	LYS	CB-CG-CD	7.52	128.59	111.30
1	2	274	GLY	N-CA-C	7.52	125.75	115.30
1	4	189	LEU	CA-C-N	7.52	129.68	120.51
1	4	189	LEU	C-N-CA	7.52	129.68	120.51
1	4	217	GLN	CA-CB-CG	7.51	129.13	114.10
1	4	44	LEU	O-C-N	7.51	129.81	122.07
1	4	266	ALA	CA-C-O	-7.50	111.63	120.10
1	2	114	LEU	CB-CG-CD2	7.47	133.12	110.70
1	4	299	LYS	CA-CB-CG	7.47	129.04	114.10
1	1	207	HIS	CA-CB-CG	7.45	121.25	113.80
1	2	327	SER	CA-CB-OG	-7.45	96.21	111.10
1	3	268	GLN	OE1-CD-NE2	-7.44	115.16	122.60
1	1	298	ASP	O-C-N	7.44	130.63	122.15
1	3	17	THR	CA-CB-OG1	-7.43	98.46	109.60
1	2	11	ASN	CA-C-N	-7.41	112.84	123.06
1	2	11	ASN	C-N-CA	-7.41	112.84	123.06
1	1	135	ASP	CA-C-N	7.41	128.16	119.94
1	1	135	ASP	C-N-CA	7.41	128.16	119.94
1	1	300	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	4	273	THR	CB-CA-C	7.40	124.17	110.11
1	2	263	LEU	O-C-N	7.40	130.47	122.34
1	2	174	SER	CA-C-O	-7.39	110.56	118.77
1	2	314	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	4	326	ASP	CA-C-N	7.39	130.50	120.38
1	4	326	ASP	C-N-CA	7.39	130.50	120.38
1	4	201	ARG	CD-NE-CZ	7.38	134.74	124.40
1	1	153	ARG	NE-CZ-NH2	-7.37	112.57	119.20
1	1	226	ILE	N-CA-C	7.37	118.42	108.11
1	1	131	ALA	N-CA-CB	7.36	120.89	110.36
1	4	115	ASN	CB-CG-OD1	7.36	135.52	120.80
1	2	330	LEU	N-CA-CB	-7.35	99.35	110.01
1	1	80	LYS	O-C-N	7.34	130.01	122.09
1	2	168	GLY	O-C-N	-7.32	114.49	122.54
1	4	205	LYS	CA-C-O	-7.31	112.71	121.56
1	4	159	VAL	N-CA-CB	7.31	121.50	111.41
1	4	56	ASN	OD1-CG-ND2	7.30	129.90	122.60
1	2	191	MET	O-C-N	7.28	131.55	123.25
1	4	249	LEU	CA-C-N	-7.27	113.59	122.90
1	4	249	LEU	C-N-CA	-7.27	113.59	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	223	GLN	CB-CG-CD	7.27	124.95	112.60
1	4	139	ASN	CA-CB-CG	7.23	119.83	112.60
1	2	51	LEU	CA-C-O	7.23	128.63	120.90
1	2	121	VAL	CB-CA-C	7.22	121.32	110.63
1	2	323	LYS	CG-CD-CE	7.22	127.91	111.30
1	3	217	GLN	O-C-N	7.22	130.84	122.25
1	4	79	GLY	CA-C-O	-7.22	113.32	120.75
1	1	317	VAL	N-CA-CB	7.21	118.99	110.55
1	2	62	VAL	CA-C-O	-7.21	112.46	120.25
1	1	269	THR	CA-CB-CG2	7.20	122.73	110.50
1	4	87	ASP	CA-C-N	7.20	131.03	120.95
1	4	87	ASP	C-N-CA	7.20	131.03	120.95
1	2	72	ASN	N-CA-CB	-7.19	98.68	110.40
1	4	116	THR	CA-CB-CG2	7.18	122.71	110.50
1	4	161	MET	CA-CB-CG	-7.18	99.75	114.10
1	4	288	PHE	CA-C-N	7.17	131.33	122.37
1	4	288	PHE	C-N-CA	7.17	131.33	122.37
1	4	90	ASP	N-CA-CB	-7.17	97.85	110.39
1	2	241	LEU	O-C-N	7.16	129.82	122.09
1	4	122	VAL	CA-CB-CG1	7.15	122.56	110.40
1	3	319	LEU	CA-C-O	-7.15	112.84	120.42
1	1	319	LEU	N-CA-CB	-7.13	99.74	110.07
1	3	263	LEU	N-CA-CB	-7.12	100.28	110.81
1	1	77	LYS	O-C-N	-7.11	114.69	122.09
1	2	202	LEU	O-C-N	7.11	127.91	121.80
1	3	79	GLY	O-C-N	-7.11	115.37	122.19
1	1	336	GLU	CB-CA-C	-7.10	97.45	109.38
1	2	89	ASN	O-C-N	7.10	131.00	122.27
1	3	84	GLU	N-CA-CB	7.10	120.55	110.12
1	4	319	LEU	O-C-N	7.09	130.75	122.17
1	1	107	ALA	O-C-N	7.09	129.64	122.12
1	1	201	ARG	CD-NE-CZ	7.07	134.30	124.40
1	2	116	THR	CA-CB-CG2	7.07	122.52	110.50
1	3	317	VAL	CB-CA-C	7.06	123.67	112.16
1	4	9	LEU	N-CA-CB	-7.06	98.90	110.41
1	4	243	GLN	OE1-CD-NE2	-7.06	115.54	122.60
1	1	317	VAL	N-CA-C	7.05	117.19	110.42
1	3	290	LEU	N-CA-CB	-7.04	98.95	110.43
1	4	89	ASN	CA-C-N	7.04	135.12	121.18
1	4	89	ASN	C-N-CA	7.04	135.12	121.18
1	2	46	ALA	CA-C-N	7.04	129.16	120.22
1	2	46	ALA	C-N-CA	7.04	129.16	120.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	117	ASP	CB-CA-C	-7.03	95.53	109.67
1	4	323	LYS	CB-CG-CD	7.03	127.47	111.30
1	2	318	GLU	CG-CD-OE2	-7.03	102.24	118.40
1	2	317	VAL	CB-CA-C	-7.02	102.53	112.22
1	3	115	ASN	CB-CG-OD1	7.01	134.83	120.80
1	2	262	ARG	CB-CG-CD	7.01	127.43	111.30
1	3	271	ARG	CG-CD-NE	7.00	127.39	112.00
1	2	204	ALA	CA-C-O	-6.99	111.36	119.05
1	1	206	ARG	CB-CG-CD	-6.99	95.23	111.30
1	1	10	ALA	N-CA-CB	6.99	121.64	110.46
1	2	270	LEU	O-C-N	6.98	129.51	122.12
1	2	275	THR	CA-CB-CG2	6.97	122.36	110.50
1	2	264	THR	CB-CA-C	6.97	125.36	112.05
1	3	224	VAL	O-C-N	6.97	130.73	123.20
1	4	192	VAL	CB-CA-C	6.97	119.82	110.42
1	1	113	THR	CA-C-O	-6.96	110.96	119.18
1	4	243	GLN	O-C-N	6.96	130.09	122.15
1	4	291	ARG	NE-CZ-NH2	6.96	125.47	119.20
1	3	178	LYS	CA-C-O	6.95	129.14	121.56
1	1	320	ALA	N-CA-CB	6.95	120.33	110.12
1	3	77	LYS	CA-C-O	-6.94	113.53	120.82
1	1	332	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	2	9	LEU	CB-CA-C	6.93	121.20	109.50
1	2	262	ARG	CA-CB-CG	-6.92	100.25	114.10
1	4	106	THR	CA-CB-OG1	-6.92	99.21	109.60
1	1	311	GLU	CA-C-O	-6.92	112.01	119.97
1	4	95	VAL	CA-CB-CG1	6.91	122.15	110.40
1	1	276	GLN	CG-CD-NE2	-6.90	106.04	116.40
1	1	142	ASN	CA-C-O	-6.90	113.23	120.55
1	1	257	GLY	CA-C-N	6.90	130.51	120.71
1	1	257	GLY	C-N-CA	6.90	130.51	120.71
1	1	162	ASN	CA-CB-CG	6.90	119.50	112.60
1	1	295	GLN	O-C-N	6.89	126.78	121.88
1	2	70	ILE	CA-C-O	6.89	128.47	121.58
1	2	80	LYS	CA-CB-CG	-6.89	100.31	114.10
1	2	293	ALA	CA-C-O	-6.89	113.13	120.71
1	4	259	VAL	CA-C-O	-6.89	113.17	120.48
1	2	319	LEU	N-CA-CB	-6.88	100.00	109.98
1	4	155	LYS	CA-C-O	-6.88	111.13	119.32
1	4	78	LEU	CA-C-O	6.88	127.78	120.70
1	3	249	LEU	CA-C-N	-6.87	113.79	122.37
1	3	249	LEU	C-N-CA	-6.87	113.79	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	259	VAL	CA-CB-CG2	6.86	122.06	110.40
1	3	61	GLN	N-CA-CB	6.86	120.19	110.46
1	1	162	ASN	OD1-CG-ND2	6.85	129.45	122.60
1	1	77	LYS	CA-C-N	6.85	130.02	120.29
1	1	77	LYS	C-N-CA	6.85	130.02	120.29
1	4	77	LYS	CG-CD-CE	6.85	127.05	111.30
1	2	194	GLU	CA-CB-CG	6.84	127.77	114.10
1	3	61	GLN	CG-CD-NE2	6.84	126.65	116.40
1	1	275	THR	CA-C-N	-6.82	111.19	120.87
1	1	275	THR	C-N-CA	-6.82	111.19	120.87
1	2	10	ALA	N-CA-C	-6.82	101.35	110.55
1	4	82	VAL	O-C-N	-6.81	115.21	121.89
1	2	51	LEU	CA-C-N	6.80	130.30	120.38
1	2	51	LEU	C-N-CA	6.80	130.30	120.38
1	1	329	GLU	N-CA-CB	6.79	120.20	110.16
1	2	56	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	3	276	GLN	OE1-CD-NE2	-6.78	115.83	122.60
1	1	254	THR	CA-C-O	-6.77	113.82	121.81
1	3	15	LEU	O-C-N	6.77	130.94	123.22
1	2	239	LYS	CA-C-O	-6.76	113.38	120.55
1	3	50	GLU	CG-CD-OE2	-6.75	102.86	118.40
1	1	293	ALA	N-CA-CB	6.75	119.69	110.10
1	1	325	GLN	CG-CD-OE1	6.74	134.28	120.80
1	1	41	VAL	N-CA-C	6.74	116.89	110.42
1	3	95	VAL	CA-CB-CG2	6.74	121.86	110.40
1	2	318	GLU	OE1-CD-OE2	6.73	139.06	122.90
1	4	8	LYS	N-CA-CB	6.72	121.93	110.50
1	4	223	GLN	CA-C-O	-6.72	113.03	120.69
1	3	304	VAL	CB-CA-C	6.72	121.02	110.81
1	4	9	LEU	N-CA-C	-6.72	99.64	110.32
1	3	76	LEU	N-CA-C	-6.70	103.90	111.07
1	3	160	THR	CA-CB-OG1	-6.70	99.55	109.60
1	4	79	GLY	N-CA-C	-6.70	104.69	112.73
1	3	310	PRO	CA-C-O	-6.70	110.32	120.03
1	4	269	THR	CB-CA-C	6.69	122.23	110.85
1	3	97	THR	CA-CB-OG1	-6.69	99.57	109.60
1	3	312	LYS	CB-CG-CD	6.69	126.68	111.30
1	2	15	LEU	CA-C-O	-6.68	113.59	120.54
1	2	60	GLU	CG-CD-OE2	-6.68	103.03	118.40
1	1	224	VAL	CA-C-O	-6.67	113.19	120.67
1	4	220	SER	CA-C-O	-6.67	114.13	121.33
1	1	172	SER	CA-C-O	-6.66	113.34	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	275	THR	CA-C-O	-6.66	113.10	120.69
1	4	75	LEU	CA-C-O	-6.65	113.85	120.70
1	3	238	TYR	O-C-N	6.65	128.95	122.03
1	2	291	ARG	CA-C-O	-6.65	113.88	121.19
1	1	293	ALA	O-C-N	6.65	129.95	122.11
1	2	196	LYS	CA-C-N	6.65	131.56	122.19
1	2	196	LYS	C-N-CA	6.65	131.56	122.19
1	2	269	THR	N-CA-CB	6.65	120.10	110.20
1	4	175	ILE	O-C-N	6.64	130.43	123.26
1	3	201	ARG	NE-CZ-NH2	-6.64	113.23	119.20
1	3	254	THR	N-CA-C	-6.64	101.59	110.55
1	1	297	ASP	CA-CB-CG	-6.63	105.97	112.60
1	2	310	PRO	CB-CA-C	6.63	122.50	111.56
1	4	240	ALA	CA-C-O	-6.63	113.52	120.55
1	2	109	PHE	CA-C-O	-6.62	114.05	121.00
1	3	244	ASN	CB-CG-ND2	-6.62	106.46	116.40
1	3	274	GLY	N-CA-C	6.62	124.77	115.43
1	1	244	ASN	CB-CG-OD1	6.61	134.03	120.80
1	4	222	PRO	N-CA-CB	6.59	109.09	103.35
1	1	318	GLU	CG-CD-OE2	-6.58	103.27	118.40
1	4	319	LEU	N-CA-CB	-6.58	100.40	110.13
1	1	262	ARG	CA-C-O	6.58	127.53	119.11
1	3	334	PHE	CA-CB-CG	-6.58	107.22	113.80
1	3	191	MET	CA-C-O	-6.57	113.75	121.44
1	4	223	GLN	OE1-CD-NE2	6.57	129.17	122.60
1	1	254	THR	N-CA-C	-6.57	101.68	110.55
1	2	284	ASN	CA-CB-CG	6.57	119.17	112.60
1	1	200	PHE	CA-CB-CG	-6.56	107.24	113.80
1	2	159	VAL	CA-CB-CG1	6.56	121.56	110.40
1	3	58	ARG	O-C-N	-6.56	115.67	123.27
1	1	109	PHE	CA-C-N	6.54	129.05	120.28
1	1	109	PHE	C-N-CA	6.54	129.05	120.28
1	2	115	ASN	CA-C-N	6.54	133.59	121.62
1	2	115	ASN	C-N-CA	6.54	133.59	121.62
1	4	149	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	2	279	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	4	194	GLU	CB-CG-CD	6.52	123.68	112.60
1	1	300	ASN	CB-CG-ND2	6.52	126.17	116.40
1	2	97	THR	CB-CA-C	6.52	120.28	109.53
1	4	11	ASN	O-C-N	6.52	131.34	123.13
1	4	11	ASN	CB-CG-ND2	6.52	126.17	116.40
1	4	55	ALA	N-CA-CB	-6.52	100.62	111.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	279	ARG	CD-NE-CZ	6.51	133.52	124.40
1	3	64	GLN	CB-CG-CD	6.51	123.66	112.60
1	2	297	ASP	O-C-N	6.50	129.01	122.12
1	2	289	VAL	CB-CA-C	6.49	118.81	110.96
1	3	236	THR	CA-C-O	-6.49	114.01	120.82
1	3	121	VAL	CB-CA-C	6.48	120.22	110.63
1	3	318	GLU	CB-CA-C	-6.47	100.04	110.79
1	4	199	TRP	CA-C-O	-6.47	113.38	120.43
1	1	322	VAL	N-CA-C	-6.46	103.52	112.50
1	4	186	TRP	CA-C-N	6.45	132.00	121.87
1	4	186	TRP	C-N-CA	6.45	132.00	121.87
1	1	314	ARG	CA-C-O	-6.45	114.05	120.82
1	1	210	ASN	O-C-N	-6.45	114.58	122.25
1	3	273	THR	O-C-N	-6.45	114.07	122.39
1	1	243	GLN	N-CA-CB	6.45	120.15	110.22
1	2	115	ASN	CB-CG-OD1	6.44	133.68	120.80
1	1	317	VAL	CB-CA-C	-6.44	103.73	111.97
1	4	203	PRO	CA-C-O	6.42	129.51	121.67
1	4	109	PHE	O-C-N	6.42	128.68	122.07
1	2	72	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	1	335	TRP	CA-C-O	-6.41	111.55	119.18
1	4	196	LYS	CA-C-O	-6.41	113.69	120.80
1	1	64	GLN	CB-CA-C	6.40	121.03	111.17
1	1	331	GLN	OE1-CD-NE2	6.40	129.00	122.60
1	3	332	ARG	N-CA-C	-6.40	104.39	111.36
1	3	81	ARG	NE-CZ-NH1	-6.39	115.11	121.50
1	3	176	ASN	OD1-CG-ND2	6.39	128.99	122.60
1	1	150	LYS	CA-C-O	-6.39	111.76	119.49
1	1	123	VAL	CG1-CB-CG2	6.38	124.85	110.80
1	2	157	VAL	CA-C-O	-6.38	114.41	121.23
1	1	132	MET	CB-CA-C	6.38	120.55	109.65
1	3	323	LYS	CB-CG-CD	6.38	125.97	111.30
1	4	332	ARG	CA-C-O	-6.37	114.13	120.82
1	4	311	GLU	CA-CB-CG	6.37	126.83	114.10
1	3	179	THR	N-CA-CB	-6.36	99.83	110.39
1	3	300	ASN	CA-CB-CG	6.36	118.96	112.60
1	1	115	ASN	CB-CG-OD1	-6.36	108.08	120.80
1	2	9	LEU	N-CA-CB	-6.36	100.27	110.63
1	1	202	LEU	O-C-N	6.35	126.50	121.55
1	3	179	THR	CB-CA-C	6.35	123.58	110.31
1	3	318	GLU	CG-CD-OE2	-6.35	103.79	118.40
1	1	196	LYS	CB-CA-C	-6.34	97.96	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	46	ALA	CA-C-N	6.34	128.27	120.22
1	4	46	ALA	C-N-CA	6.34	128.27	120.22
1	3	180	GLU	CA-C-N	6.33	129.06	120.38
1	3	180	GLU	C-N-CA	6.33	129.06	120.38
1	2	271	ARG	CA-C-O	6.33	127.46	120.82
1	4	284	ASN	OD1-CG-ND2	6.33	128.93	122.60
1	3	258	SER	CA-C-N	-6.32	114.20	122.99
1	3	258	SER	C-N-CA	-6.32	114.20	122.99
1	4	115	ASN	O-C-N	-6.32	114.19	122.59
1	2	336	GLU	CA-C-O	-6.31	112.22	118.97
1	1	100	THR	CA-C-N	6.30	129.05	120.54
1	1	100	THR	C-N-CA	6.30	129.05	120.54
1	1	100	THR	CA-CB-OG1	-6.30	100.14	109.60
1	1	174	SER	CA-C-N	6.30	131.49	123.10
1	1	174	SER	C-N-CA	6.30	131.49	123.10
1	4	159	VAL	CA-CB-CG2	6.30	121.11	110.40
1	4	64	GLN	CB-CG-CD	6.30	123.30	112.60
1	1	263	LEU	CB-CG-CD2	-6.29	91.82	110.70
1	2	277	ILE	CA-C-O	-6.29	113.30	120.66
1	1	191	MET	CA-C-N	6.29	131.46	123.10
1	1	191	MET	C-N-CA	6.29	131.46	123.10
1	4	101	ASP	N-CA-C	6.29	118.94	111.33
1	1	182	PHE	O-C-N	-6.28	115.29	123.02
1	2	329	GLU	CB-CA-C	-6.28	100.17	110.85
1	3	16	ALA	CA-C-O	-6.28	113.45	120.54
1	1	263	LEU	CB-CA-C	-6.27	98.53	109.07
1	2	142	ASN	CA-C-O	-6.27	112.39	119.79
1	3	164	GLU	O-C-N	6.27	131.51	123.11
1	4	150	LYS	CA-C-O	6.27	127.19	120.10
1	4	64	GLN	N-CA-CB	6.27	122.89	111.11
1	3	249	LEU	CA-C-O	-6.26	113.60	120.36
1	2	160	THR	CA-CB-CG2	6.26	121.14	110.50
1	2	271	ARG	NE-CZ-NH1	6.26	127.76	121.50
1	3	304	VAL	N-CA-CB	-6.25	99.64	111.21
1	4	12	VAL	CA-CB-CG1	6.25	121.03	110.40
1	3	150	LYS	CA-CB-CG	6.25	126.60	114.10
1	1	159	VAL	N-CA-CB	6.25	120.03	111.41
1	3	57	VAL	N-CA-C	6.25	117.29	108.36
1	3	272	LYS	N-CA-CB	6.25	119.43	110.06
1	2	180	GLU	CB-CG-CD	6.25	123.22	112.60
1	2	279	ARG	CG-CD-NE	6.25	125.74	112.00
1	4	79	GLY	O-C-N	6.25	128.19	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	289	VAL	CA-C-N	6.24	131.00	122.19
1	4	289	VAL	C-N-CA	6.24	131.00	122.19
1	3	151	ASP	CA-C-O	-6.24	111.94	119.49
1	3	262	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	1	74	ASP	CA-CB-CG	6.24	118.84	112.60
1	2	78	LEU	O-C-N	6.24	129.26	122.15
1	4	232	ASN	CA-CB-CG	6.24	118.84	112.60
1	2	76	LEU	O-C-N	6.23	128.57	122.09
1	2	133	SER	CA-C-N	6.23	129.61	120.82
1	2	133	SER	C-N-CA	6.23	129.61	120.82
1	3	328	LYS	CA-C-N	6.23	129.14	120.29
1	3	328	LYS	C-N-CA	6.23	129.14	120.29
1	1	292	ASN	CB-CG-OD1	6.23	133.26	120.80
1	1	87	ASP	CB-CG-OD2	-6.23	104.08	118.40
1	2	236	THR	N-CA-C	6.22	118.61	111.02
1	4	254	THR	N-CA-C	-6.22	102.15	110.55
1	4	206	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	2	263	LEU	CD1-CG-CD2	6.22	124.48	110.80
1	3	266	ALA	CA-C-O	-6.21	112.82	119.97
1	1	98	HIS	CA-C-N	6.20	125.87	119.92
1	1	98	HIS	C-N-CA	6.20	125.87	119.92
1	2	304	VAL	CG1-CB-CG2	6.20	124.43	110.80
1	1	84	GLU	CB-CG-CD	6.18	123.11	112.60
1	4	155	LYS	O-C-N	6.18	129.72	122.24
1	4	99	GLY	N-CA-C	-6.18	104.17	112.14
1	1	136	GLY	N-CA-C	6.18	119.66	112.50
1	4	329	GLU	CA-C-O	6.17	126.96	120.42
1	1	304	VAL	CG1-CB-CG2	6.17	124.37	110.80
1	2	153	ARG	NE-CZ-NH2	-6.17	113.65	119.20
1	4	298	ASP	O-C-N	6.16	128.41	122.07
1	3	182	PHE	N-CA-C	6.16	118.22	108.67
1	4	197	SER	CA-C-O	-6.16	113.96	120.80
1	3	86	ALA	N-CA-C	-6.15	104.58	111.28
1	3	129	GLY	N-CA-C	6.14	121.44	113.27
1	1	84	GLU	CA-C-N	6.14	129.01	120.29
1	1	84	GLU	C-N-CA	6.14	129.01	120.29
1	2	58	ARG	O-C-N	6.14	130.76	123.33
1	2	233	VAL	CG1-CB-CG2	6.14	124.30	110.80
1	2	100	THR	CA-CB-CG2	6.13	120.93	110.50
1	4	332	ARG	NH1-CZ-NH2	6.13	127.26	119.30
1	4	327	SER	CA-CB-OG	-6.12	98.86	111.10
1	4	64	GLN	O-C-N	6.11	131.37	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	17	THR	CA-CB-OG1	-6.11	100.43	109.60
1	1	186	TRP	CA-C-N	6.11	131.47	121.87
1	1	186	TRP	C-N-CA	6.11	131.47	121.87
1	4	273	THR	OG1-CB-CG2	-6.11	97.08	109.30
1	4	261	SER	CA-CB-OG	-6.11	98.89	111.10
1	4	105	GLU	CA-C-O	-6.10	114.02	120.55
1	4	98	HIS	N-CA-CB	-6.10	100.19	111.53
1	3	58	ARG	CB-CA-C	6.09	123.09	109.56
1	2	330	LEU	CB-CA-C	6.09	120.44	110.88
1	1	207	HIS	CA-C-O	-6.08	114.93	121.38
1	1	74	ASP	N-CA-C	-6.08	104.77	111.82
1	2	218	ILE	CA-C-O	-6.08	114.07	120.57
1	1	13	VAL	CB-CA-C	6.08	119.88	110.83
1	3	162	ASN	CB-CG-OD1	-6.07	108.65	120.80
1	3	299	LYS	CA-C-O	-6.07	113.98	120.42
1	4	223	GLN	O-C-N	6.07	130.14	123.04
1	2	189	LEU	N-CA-C	-6.07	104.95	112.90
1	1	306	HIS	CA-CB-CG	-6.06	107.74	113.80
1	3	221	LEU	CB-CA-C	6.06	117.06	108.76
1	1	314	ARG	O-C-N	6.05	128.30	122.07
1	4	213	PHE	O-C-N	6.05	130.78	123.16
1	2	100	THR	CA-CB-OG1	-6.05	100.53	109.60
1	2	224	VAL	CA-C-O	-6.05	113.95	120.36
1	1	115	ASN	N-CA-CB	6.04	120.04	110.49
1	3	170	ASP	CA-C-O	-6.04	112.46	119.59
1	4	148	SER	CA-CB-OG	-6.04	99.02	111.10
1	2	72	ASN	O-C-N	-6.03	114.14	122.46
1	2	233	VAL	O-C-N	6.03	129.03	122.57
1	4	258	SER	CA-C-N	-6.03	115.71	123.19
1	4	258	SER	C-N-CA	-6.03	115.71	123.19
1	4	317	VAL	N-CA-CB	6.03	119.63	110.58
1	3	325	GLN	N-CA-C	-6.02	104.05	113.02
1	1	309	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	3	17	THR	CA-CB-CG2	6.02	120.74	110.50
1	3	148	SER	CB-CA-C	-6.02	97.40	109.99
1	3	270	LEU	CA-C-N	6.02	128.27	120.44
1	3	270	LEU	C-N-CA	6.02	128.27	120.44
1	3	276	GLN	CG-CD-OE1	6.02	132.84	120.80
1	3	137	MET	CB-CA-C	6.02	120.78	110.79
1	3	239	LYS	CD-CE-NZ	6.02	131.15	111.90
1	2	326	ASP	CA-C-N	6.01	128.94	120.28
1	2	326	ASP	C-N-CA	6.01	128.94	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	291	ARG	N-CA-CB	6.01	118.89	109.69
1	4	284	ASN	N-CA-C	6.01	120.74	113.17
1	4	290	LEU	CA-CB-CG	6.00	137.31	116.30
1	2	325	GLN	CG-CD-NE2	6.00	125.40	116.40
1	2	188	PRO	CB-CA-C	-5.99	103.10	110.95
1	1	228	TYR	CA-C-O	-5.99	114.15	120.80
1	3	118	LYS	O-C-N	5.99	128.14	121.43
1	1	271	ARG	NE-CZ-NH1	5.99	127.49	121.50
1	3	322	VAL	CA-C-N	5.99	133.01	122.42
1	3	322	VAL	C-N-CA	5.99	133.01	122.42
1	4	66	ALA	N-CA-C	-5.98	98.98	108.73
1	1	79	GLY	CA-C-N	5.97	128.57	120.44
1	1	79	GLY	C-N-CA	5.97	128.57	120.44
1	3	135	ASP	CA-C-O	5.97	126.25	119.27
1	1	318	GLU	CB-CA-C	-5.96	100.89	110.79
1	3	161	MET	O-C-N	5.96	130.93	123.19
1	2	260	SER	CA-C-O	5.95	127.74	121.19
1	4	169	ARG	CA-C-N	-5.95	113.31	122.60
1	4	169	ARG	C-N-CA	-5.95	113.31	122.60
1	4	55	ALA	N-CA-C	5.95	117.19	108.14
1	3	9	LEU	CA-C-O	-5.95	113.59	120.31
1	1	156	GLY	CA-C-O	-5.94	113.51	122.71
1	1	132	MET	N-CA-CB	-5.93	101.25	109.97
1	3	74	ASP	N-CA-C	-5.93	104.94	111.82
1	4	246	ALA	CA-C-O	-5.93	114.67	121.19
1	1	270	LEU	CB-CA-C	5.93	120.63	110.79
1	2	60	GLU	O-C-N	5.92	130.34	123.41
1	2	197	SER	CA-C-O	-5.92	113.85	120.54
1	1	58	ARG	N-CA-CB	5.92	121.20	111.08
1	1	144	VAL	CA-C-N	5.92	128.53	120.54
1	1	144	VAL	C-N-CA	5.92	128.53	120.54
1	2	317	VAL	CA-C-O	-5.92	114.58	120.85
1	1	163	ASP	O-C-N	5.91	129.39	122.00
1	2	101	ASP	CB-CG-OD1	5.91	131.99	118.40
1	3	251	HIS	CA-CB-CG	5.90	119.70	113.80
1	3	58	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	4	127	ARG	NE-CZ-NH1	5.90	127.40	121.50
1	2	60	GLU	CA-CB-CG	5.90	125.90	114.10
1	3	47	GLY	N-CA-C	-5.90	107.35	114.66
1	3	239	LYS	CG-CD-CE	5.87	124.81	111.30
1	2	236	THR	CA-CB-OG1	-5.87	100.80	109.60
1	1	103	LEU	CA-CB-CG	5.86	136.82	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	263	LEU	CA-CB-CG	-5.86	95.78	116.30
1	4	181	ALA	CA-C-O	-5.86	114.30	120.63
1	2	309	ASN	CA-CB-CG	5.86	118.46	112.60
1	4	219	SER	O-C-N	5.86	129.06	122.27
1	4	309	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	3	45	ILE	CA-C-N	5.86	130.50	120.72
1	3	45	ILE	C-N-CA	5.86	130.50	120.72
1	1	137	MET	CA-CB-CG	-5.85	102.40	114.10
1	1	165	ILE	CA-C-O	-5.85	113.08	120.86
1	3	179	THR	CA-CB-CG2	5.85	120.45	110.50
1	1	91	VAL	O-C-N	5.85	129.26	123.18
1	1	97	THR	CA-C-O	5.85	127.15	120.54
1	1	297	ASP	CA-C-O	-5.85	113.24	119.97
1	4	273	THR	O-C-N	-5.84	113.74	122.39
1	4	142	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	4	173	LYS	N-CA-C	-5.84	99.62	108.67
1	4	103	LEU	O-C-N	-5.83	115.94	122.12
1	4	90	ASP	CB-CA-C	-5.83	98.29	110.17
1	3	331	GLN	CB-CG-CD	5.82	122.49	112.60
1	1	273	THR	CA-C-N	5.81	131.47	121.07
1	1	273	THR	C-N-CA	5.81	131.47	121.07
1	4	48	VAL	N-CA-CB	5.81	119.34	111.21
1	3	95	VAL	O-C-N	5.81	129.45	123.18
1	4	18	GLY	CA-C-O	5.81	128.13	121.05
1	4	119	PRO	CA-C-O	-5.81	115.02	121.23
1	2	289	VAL	CA-C-N	5.80	130.37	122.19
1	2	289	VAL	C-N-CA	5.80	130.37	122.19
1	3	240	ALA	N-CA-C	5.80	117.61	111.28
1	1	110	LEU	O-C-N	-5.80	115.97	122.12
1	2	50	GLU	CA-C-N	5.79	128.36	120.54
1	2	50	GLU	C-N-CA	5.79	128.36	120.54
1	3	148	SER	CA-C-N	5.79	130.11	122.30
1	3	148	SER	C-N-CA	5.79	130.11	122.30
1	3	273	THR	CB-CA-C	5.78	120.66	110.37
1	1	289	VAL	CB-CA-C	5.78	118.08	110.91
1	1	263	LEU	O-C-N	5.78	129.47	122.48
1	3	270	LEU	N-CA-CB	-5.78	101.63	110.12
1	3	203	PRO	CA-C-O	-5.77	114.63	121.67
1	4	82	VAL	CB-CA-C	5.77	119.60	112.04
1	3	241	LEU	N-CA-CB	-5.77	101.64	110.12
1	2	198	TYR	CA-C-O	-5.76	114.13	120.24
1	4	125	SER	CB-CA-C	-5.76	97.68	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	11	ASN	CA-CB-CG	5.76	118.36	112.60
1	1	105	GLU	CA-C-N	5.76	128.00	120.28
1	1	105	GLU	C-N-CA	5.76	128.00	120.28
1	4	57	VAL	N-CA-CB	-5.75	103.44	111.25
1	1	170	ASP	CA-C-O	-5.74	112.81	119.59
1	4	140	LEU	O-C-N	5.74	128.70	122.15
1	4	206	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	3	289	VAL	CA-CB-CG2	5.74	120.15	110.40
1	4	68	GLU	CB-CG-CD	5.74	122.35	112.60
1	4	107	ALA	CA-C-N	5.74	128.43	120.29
1	4	107	ALA	C-N-CA	5.74	128.43	120.29
1	2	275	THR	CA-CB-OG1	-5.73	101.00	109.60
1	2	333	ILE	CA-C-N	5.73	129.77	120.60
1	2	333	ILE	C-N-CA	5.73	129.77	120.60
1	1	143	ALA	N-CA-CB	5.73	118.32	110.01
1	1	235	ASP	CA-CB-CG	5.73	118.33	112.60
1	4	148	SER	CB-CA-C	-5.73	98.01	109.99
1	2	285	GLN	CA-C-N	5.73	130.14	120.86
1	2	285	GLN	C-N-CA	5.73	130.14	120.86
1	4	323	LYS	CA-CB-CG	5.73	125.56	114.10
1	1	312	LYS	N-CA-C	-5.72	104.65	111.69
1	1	259	VAL	CB-CA-C	5.72	119.09	110.63
1	3	329	GLU	CA-C-N	5.71	127.94	120.28
1	3	329	GLU	C-N-CA	5.71	127.94	120.28
1	2	285	GLN	OE1-CD-NE2	5.71	128.31	122.60
1	4	90	ASP	N-CA-C	5.71	119.86	113.01
1	1	11	ASN	O-C-N	5.71	129.84	123.05
1	3	218	ILE	O-C-N	5.70	129.77	123.10
1	3	184	SER	CA-C-O	-5.70	114.44	121.11
1	4	256	ASN	CA-CB-CG	-5.70	106.90	112.60
1	2	233	VAL	CA-CB-CG2	5.70	120.09	110.40
1	1	317	VAL	O-C-N	5.69	127.49	121.91
1	1	141	TYR	CA-C-N	5.69	127.91	120.28
1	1	141	TYR	C-N-CA	5.69	127.91	120.28
1	1	76	LEU	CA-C-O	-5.69	114.84	120.70
1	1	244	ASN	CA-C-O	-5.69	112.55	119.43
1	4	43	LYS	N-CA-C	-5.69	105.08	111.28
1	4	178	LYS	N-CA-CB	-5.68	101.98	110.17
1	3	308	LEU	CA-C-O	-5.68	114.28	120.81
1	4	136	GLY	CA-C-N	5.68	128.14	120.65
1	4	136	GLY	C-N-CA	5.68	128.14	120.65
1	2	56	ASN	N-CA-C	-5.67	99.28	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	60	GLU	CB-CG-CD	5.67	122.24	112.60
1	1	113	THR	CA-CB-CG2	5.67	120.13	110.50
1	2	74	ASP	CA-CB-CG	5.66	118.26	112.60
1	1	106	THR	CA-CB-OG1	-5.66	101.11	109.60
1	4	71	THR	CA-C-N	5.66	128.43	120.28
1	4	71	THR	C-N-CA	5.66	128.43	120.28
1	2	262	ARG	CD-NE-CZ	-5.66	116.48	124.40
1	3	327	SER	CA-CB-OG	-5.66	99.79	111.10
1	4	56	ASN	CA-CB-CG	-5.66	106.94	112.60
1	1	87	ASP	O-C-N	5.65	130.68	122.43
1	1	176	ASN	CB-CG-ND2	-5.64	107.94	116.40
1	2	166	GLN	CG-CD-NE2	5.64	124.86	116.40
1	2	52	ALA	O-C-N	5.64	128.63	122.20
1	4	229	SER	N-CA-CB	-5.64	101.44	111.08
1	4	48	VAL	CA-C-O	5.63	127.50	119.95
1	3	121	VAL	CA-CB-CG1	5.63	119.98	110.40
1	4	83	ALA	O-C-N	5.63	128.09	122.12
1	1	75	LEU	CB-CA-C	5.63	119.79	110.90
1	2	76	LEU	N-CA-CB	5.62	118.32	109.94
1	2	82	VAL	O-C-N	5.62	127.62	121.83
1	4	243	GLN	CA-CB-CG	5.62	125.34	114.10
1	1	279	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	3	71	THR	CA-CB-CG2	5.62	120.05	110.50
1	3	101	ASP	CA-C-O	-5.62	114.60	120.55
1	3	289	VAL	N-CA-CB	5.62	116.84	110.72
1	4	77	LYS	O-C-N	5.62	127.86	122.07
1	3	331	GLN	N-CA-CB	5.60	118.45	110.16
1	1	171	VAL	CA-C-O	-5.60	115.82	121.59
1	1	309	ASN	CB-CG-ND2	5.60	124.80	116.40
1	3	169	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
1	3	74	ASP	CA-C-O	-5.60	113.53	119.97
1	1	299	LYS	CA-C-O	-5.59	114.94	120.70
1	4	272	LYS	CA-C-O	5.59	126.67	120.63
1	2	299	LYS	CB-CA-C	-5.59	101.87	110.81
1	4	266	ALA	O-C-N	5.59	128.76	122.22
1	4	310	PRO	CB-CA-C	5.59	122.64	113.20
1	1	329	GLU	CB-CG-CD	5.58	122.09	112.60
1	2	55	ALA	CA-C-O	-5.58	115.33	121.31
1	3	186	TRP	CA-C-N	5.58	130.63	121.87
1	3	186	TRP	C-N-CA	5.58	130.63	121.87
1	1	320	ALA	N-CA-C	-5.58	105.20	111.28
1	4	232	ASN	OD1-CG-ND2	-5.58	117.02	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	190	GLY	O-C-N	5.58	129.88	123.58
1	1	270	LEU	N-CA-CB	-5.57	101.93	110.12
1	2	161	MET	CA-CB-CG	-5.57	102.95	114.10
1	2	262	ARG	NH1-CZ-NH2	5.57	126.54	119.30
1	3	113	THR	N-CA-C	5.57	121.86	114.12
1	1	146	VAL	CA-C-N	5.56	128.29	120.28
1	1	146	VAL	C-N-CA	5.56	128.29	120.28
1	1	52	ALA	CA-C-O	-5.56	113.05	119.61
1	2	13	VAL	CA-CB-CG2	-5.55	100.96	110.40
1	1	284	ASN	CA-CB-CG	5.55	118.15	112.60
1	1	138	LEU	CA-C-O	-5.55	114.67	120.55
1	2	264	THR	CA-C-N	5.55	125.01	119.24
1	2	264	THR	C-N-CA	5.55	125.01	119.24
1	2	303	VAL	CA-C-O	-5.54	114.85	121.28
1	3	245	GLY	CA-C-O	-5.54	112.43	119.19
1	2	117	ASP	CB-CA-C	5.54	119.53	110.17
1	1	239	LYS	CB-CG-CD	-5.54	98.56	111.30
1	3	273	THR	CA-C-O	5.54	126.13	119.43
1	4	296	PRO	N-CA-CB	-5.54	98.89	102.65
1	4	314	ARG	CD-NE-CZ	5.53	132.15	124.40
1	2	277	ILE	O-C-N	5.53	130.12	122.88
1	1	73	ASP	O-C-N	5.53	129.07	122.27
1	1	193	VAL	O-C-N	5.53	128.39	123.03
1	1	206	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	3	143	ALA	N-CA-C	-5.53	105.16	111.07
1	1	336	GLU	CB-CG-CD	5.52	121.99	112.60
1	3	99	GLY	N-CA-C	-5.52	105.02	112.14
1	4	153	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	3	237	ALA	O-C-N	-5.51	115.87	122.15
1	4	66	ALA	CB-CA-C	5.50	119.11	110.19
1	1	153	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	1	272	LYS	CB-CA-C	5.50	120.81	110.63
1	2	218	ILE	O-C-N	5.50	129.14	123.03
1	4	236	THR	N-CA-C	5.50	117.71	111.11
1	2	244	ASN	CB-CA-C	5.50	120.01	110.94
1	1	303	VAL	CB-CA-C	5.49	119.28	110.82
1	2	186	TRP	CA-C-N	5.49	130.49	121.87
1	2	186	TRP	C-N-CA	5.49	130.49	121.87
1	1	174	SER	N-CA-CB	-5.49	103.04	110.67
1	1	276	GLN	N-CA-CB	-5.49	101.90	109.97
1	4	214	ASP	CB-CG-OD2	-5.49	105.78	118.40
1	3	239	LYS	CA-C-N	5.49	127.63	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	239	LYS	C-N-CA	5.49	127.63	120.28
1	2	58	ARG	CA-CB-CG	5.48	125.06	114.10
1	4	146	VAL	CA-C-N	5.48	128.17	120.28
1	4	146	VAL	C-N-CA	5.48	128.17	120.28
1	4	214	ASP	CB-CG-OD1	5.48	131.01	118.40
1	2	209	VAL	N-CA-C	5.48	118.73	111.17
1	1	15	LEU	CA-C-O	-5.48	114.84	120.54
1	2	114	LEU	O-C-N	-5.47	115.32	122.43
1	4	165	ILE	N-CA-C	-5.47	99.27	107.37
1	1	51	LEU	O-C-N	5.47	127.78	122.09
1	4	274	GLY	CA-C-O	-5.47	112.94	119.01
1	4	223	GLN	CG-CD-OE1	-5.46	109.88	120.80
1	4	182	PHE	N-CA-C	5.46	117.60	109.25
1	1	154	GLY	N-CA-C	5.45	122.88	115.30
1	3	121	VAL	CA-CB-CG2	5.45	119.66	110.40
1	1	334	PHE	CA-CB-CG	-5.45	108.35	113.80
1	1	291	ARG	CD-NE-CZ	5.45	132.02	124.40
1	4	161	MET	CA-C-N	-5.44	114.52	122.19
1	4	161	MET	C-N-CA	-5.44	114.52	122.19
1	4	333	ILE	N-CA-CB	-5.44	103.14	110.54
1	1	11	ASN	CA-C-N	-5.43	116.45	123.19
1	1	11	ASN	C-N-CA	-5.43	116.45	123.19
1	2	138	LEU	CA-C-O	-5.43	114.67	120.42
1	1	241	LEU	N-CA-C	-5.43	105.39	112.23
1	3	268	GLN	CA-CB-CG	-5.43	103.25	114.10
1	1	82	VAL	N-CA-C	-5.42	105.24	110.72
1	2	180	GLU	CA-C-O	5.42	126.25	119.59
1	4	11	ASN	CA-C-O	-5.42	114.66	120.46
1	1	327	SER	N-CA-C	5.41	117.88	111.33
1	2	111	ASP	CA-CB-CG	5.41	118.01	112.60
1	2	115	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	2	42	ASP	N-CA-CB	5.40	118.25	110.20
1	3	89	ASN	CB-CG-OD1	-5.40	110.00	120.80
1	4	207	HIS	O-C-N	5.40	128.77	122.99
1	1	107	ALA	CA-C-O	-5.40	114.83	120.55
1	1	323	LYS	CA-C-O	-5.39	112.32	119.06
1	1	299	LYS	N-CA-CB	5.39	117.89	110.07
1	1	160	THR	CA-CB-OG1	-5.39	101.52	109.60
1	1	250	ILE	N-CA-CB	5.39	117.52	111.21
1	2	280	SER	O-C-N	-5.38	116.92	122.84
1	3	89	ASN	CA-C-O	5.38	126.16	119.97
1	4	218	ILE	CA-C-N	-5.38	113.78	122.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	218	ILE	C-N-CA	-5.38	113.78	122.23
1	4	269	THR	CA-C-N	5.38	127.93	120.29
1	4	269	THR	C-N-CA	5.38	127.93	120.29
1	1	82	VAL	CA-C-O	-5.38	115.15	120.85
1	3	179	THR	OG1-CB-CG2	5.38	120.05	109.30
1	1	182	PHE	CA-C-N	5.37	131.00	122.62
1	1	182	PHE	C-N-CA	5.37	131.00	122.62
1	2	233	VAL	CA-C-O	-5.37	116.06	121.59
1	1	318	GLU	CG-CD-OE1	5.37	130.75	118.40
1	2	101	ASP	CA-CB-CG	5.37	117.97	112.60
1	2	160	THR	CA-CB-OG1	-5.37	101.55	109.60
1	3	80	LYS	CB-CA-C	-5.37	99.43	110.38
1	3	330	LEU	CA-C-N	5.37	127.91	120.29
1	3	330	LEU	C-N-CA	5.37	127.91	120.29
1	4	239	LYS	CA-CB-CG	-5.37	103.37	114.10
1	1	119	PRO	O-C-N	5.36	129.18	123.01
1	3	236	THR	CA-CB-CG2	5.36	119.61	110.50
1	3	117	ASP	CA-C-O	-5.36	113.04	119.15
1	3	329	GLU	CG-CD-OE1	5.35	130.71	118.40
1	1	166	GLN	CG-CD-NE2	5.35	124.43	116.40
1	3	189	LEU	N-CA-CB	-5.35	102.06	110.30
1	2	70	ILE	O-C-N	-5.35	117.11	122.62
1	3	15	LEU	CA-C-O	-5.35	114.64	120.36
1	3	231	GLY	CA-C-O	5.35	126.12	121.41
1	4	304	VAL	CG1-CB-CG2	5.35	122.56	110.80
1	1	308	LEU	N-CA-C	5.35	117.98	109.96
1	1	9	LEU	CA-C-O	-5.34	115.79	121.94
1	1	262	ARG	CD-NE-CZ	5.34	131.88	124.40
1	1	258	SER	CA-C-N	-5.34	116.14	123.14
1	1	258	SER	C-N-CA	-5.34	116.14	123.14
1	4	89	ASN	CB-CG-ND2	-5.34	108.39	116.40
1	1	119	PRO	CB-CA-C	-5.34	104.92	111.64
1	1	274	GLY	O-C-N	-5.33	115.71	122.32
1	3	269	THR	CA-CB-CG2	5.33	119.56	110.50
1	2	264	THR	CA-CB-OG1	-5.33	101.61	109.60
1	4	180	GLU	CA-C-N	5.32	127.67	120.38
1	4	180	GLU	C-N-CA	5.32	127.67	120.38
1	3	331	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	2	291	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	1	289	VAL	O-C-N	-5.32	116.89	122.95
1	3	60	GLU	CA-CB-CG	5.32	124.73	114.10
1	1	57	VAL	CA-CB-CG2	5.32	119.44	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	324	THR	O-C-N	-5.31	116.74	123.17
1	1	241	LEU	N-CA-CB	-5.30	102.13	110.30
1	2	114	LEU	N-CA-CB	-5.30	102.64	110.49
1	3	40	GLY	CA-C-O	-5.30	116.81	121.58
1	2	282	HIS	N-CA-C	-5.30	106.58	112.57
1	4	270	LEU	O-C-N	5.30	128.19	122.15
1	3	64	GLN	CA-CB-CG	5.29	124.69	114.10
1	3	268	GLN	CG-CD-OE1	5.29	131.38	120.80
1	2	288	PHE	O-C-N	5.29	128.81	123.26
1	3	58	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	2	52	ALA	CA-C-O	-5.27	114.29	120.20
1	4	336	GLU	CG-CD-OE2	-5.27	106.27	118.40
1	3	244	ASN	CA-CB-CG	-5.27	107.33	112.60
1	4	121	VAL	CA-C-N	-5.27	116.65	123.19
1	4	121	VAL	C-N-CA	-5.27	116.65	123.19
1	1	182	PHE	CB-CA-C	5.27	118.93	110.29
1	1	206	ARG	CG-CD-NE	-5.27	100.41	112.00
1	2	130	THR	OG1-CB-CG2	5.27	119.84	109.30
1	2	267	LEU	CB-CA-C	5.27	119.15	110.88
1	1	236	THR	N-CA-C	5.27	117.45	111.02
1	4	137	MET	CB-CA-C	5.27	119.07	110.96
1	3	102	THR	CA-CB-OG1	-5.26	101.70	109.60
1	3	309	ASN	CB-CG-ND2	5.26	124.30	116.40
1	1	230	TYR	CA-C-N	5.26	124.97	119.92
1	1	230	TYR	C-N-CA	5.26	124.97	119.92
1	4	83	ALA	N-CA-CB	5.26	117.85	110.12
1	4	317	VAL	O-C-N	5.26	127.25	121.83
1	2	146	VAL	CA-C-O	-5.26	115.08	120.71
1	1	299	LYS	O-C-N	5.26	127.77	122.09
1	2	143	ALA	CA-C-O	5.25	126.34	120.82
1	4	174	SER	CA-C-N	-5.25	116.26	123.14
1	4	174	SER	C-N-CA	-5.25	116.26	123.14
1	2	211	SER	O-C-N	5.25	128.89	122.96
1	1	250	ILE	CA-CB-CG1	-5.25	101.48	110.40
1	1	193	VAL	N-CA-CB	5.24	118.81	112.10
1	1	227	ALA	CA-C-O	5.24	126.27	120.71
1	1	75	LEU	N-CA-CB	-5.24	102.48	110.07
1	2	252	ALA	O-C-N	-5.24	115.47	122.38
1	2	261	SER	CA-C-N	5.24	131.79	121.58
1	2	261	SER	C-N-CA	5.24	131.79	121.58
1	2	139	ASN	CB-CG-ND2	5.23	124.25	116.40
1	2	224	VAL	CB-CA-C	5.23	117.96	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	12	VAL	CB-CA-C	5.23	118.41	110.62
1	1	78	LEU	N-CA-C	-5.22	105.67	111.36
1	4	186	TRP	CA-C-O	-5.22	113.24	119.35
1	4	248	ALA	CA-C-O	-5.22	115.00	121.06
1	3	139	ASN	CA-CB-CG	5.22	117.82	112.60
1	1	301	ASP	CB-CA-C	5.22	118.73	111.63
1	1	282	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	2	312	LYS	CA-CB-CG	5.21	124.53	114.10
1	4	57	VAL	O-C-N	-5.21	117.71	123.18
1	4	242	ALA	CA-C-N	5.21	127.69	120.29
1	4	242	ALA	C-N-CA	5.21	127.69	120.29
1	1	90	ASP	N-CA-C	5.21	119.14	112.26
1	1	254	THR	OG1-CB-CG2	5.21	119.72	109.30
1	2	103	LEU	CB-CG-CD1	5.21	126.33	110.70
1	2	311	GLU	CA-C-N	5.21	127.69	120.29
1	2	311	GLU	C-N-CA	5.21	127.69	120.29
1	3	262	ARG	CA-C-O	5.21	125.73	119.43
1	2	216	LYS	O-C-N	5.21	127.64	122.12
1	4	147	ALA	N-CA-CB	5.21	118.24	110.22
1	1	229	SER	CA-C-O	5.20	126.22	120.71
1	3	118	LYS	CA-CB-CG	-5.20	103.69	114.10
1	4	304	VAL	N-CA-CB	-5.20	101.59	111.21
1	3	9	LEU	CB-CA-C	5.20	118.09	109.72
1	3	171	VAL	N-CA-C	-5.20	102.87	109.58
1	3	214	ASP	O-C-N	5.20	129.94	123.28
1	4	106	THR	CA-CB-CG2	5.20	119.34	110.50
1	3	58	ARG	CB-CG-CD	5.20	123.25	111.30
1	4	221	LEU	CA-C-N	5.20	125.13	119.78
1	4	221	LEU	C-N-CA	5.20	125.13	119.78
1	4	250	ILE	CA-C-O	-5.20	114.92	120.59
1	1	294	GLU	CG-CD-OE2	5.20	130.35	118.40
1	4	60	GLU	CA-CB-CG	5.20	124.49	114.10
1	3	271	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
1	1	87	ASP	N-CA-C	5.19	119.46	113.18
1	1	269	THR	CA-CB-OG1	-5.19	101.82	109.60
1	4	80	LYS	CB-CG-CD	5.19	123.23	111.30
1	4	84	GLU	N-CA-CB	5.18	117.53	110.01
1	1	241	LEU	CB-CG-CD1	5.18	126.25	110.70
1	1	57	VAL	N-CA-C	5.18	115.42	108.17
1	1	108	TYR	N-CA-C	-5.18	105.70	112.23
1	2	219	SER	CA-CB-OG	-5.18	100.74	111.10
1	3	331	GLN	CA-C-O	-5.18	114.93	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	214	ASP	CA-C-O	-5.18	113.88	120.20
1	2	89	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	1	70	ILE	CA-C-O	-5.17	116.39	122.13
1	1	151	ASP	CA-C-O	-5.17	112.49	119.11
1	2	298	ASP	CA-C-N	5.17	127.53	120.54
1	2	298	ASP	C-N-CA	5.17	127.53	120.54
1	1	298	ASP	CA-CB-CG	-5.17	107.43	112.60
1	4	159	VAL	CB-CA-C	5.17	118.28	110.63
1	1	76	LEU	N-CA-C	-5.17	105.55	111.14
1	1	106	THR	O-C-N	5.17	127.60	122.12
1	3	198	TYR	CA-C-O	-5.17	114.76	120.24
1	1	116	THR	CA-C-N	5.17	131.03	121.52
1	1	116	THR	C-N-CA	5.17	131.03	121.52
1	1	168	GLY	O-C-N	-5.17	116.85	122.54
1	3	160	THR	CA-CB-CG2	5.16	119.27	110.50
1	4	220	SER	N-CA-CB	-5.16	103.05	111.66
1	3	236	THR	N-CA-CB	5.16	117.49	110.01
1	1	310	PRO	CA-C-N	5.16	128.15	120.31
1	1	310	PRO	C-N-CA	5.16	128.15	120.31
1	4	114	LEU	O-C-N	-5.16	116.34	122.63
1	4	322	VAL	CA-CB-CG2	5.15	119.16	110.40
1	2	61	GLN	CA-C-O	-5.15	115.56	120.92
1	3	166	GLN	CB-CG-CD	5.15	121.36	112.60
1	4	247	LYS	CA-C-O	5.15	124.81	119.14
1	3	161	MET	CA-C-O	-5.15	115.29	121.11
1	2	196	LYS	CG-CD-CE	5.14	123.13	111.30
1	3	104	GLU	CG-CD-OE2	5.14	130.23	118.40
1	3	178	LYS	CB-CA-C	5.14	119.00	109.54
1	2	48	VAL	CA-CB-CG1	5.14	119.14	110.40
1	4	178	LYS	CA-CB-CG	-5.14	103.82	114.10
1	3	101	ASP	CA-C-N	-5.14	114.46	122.37
1	3	101	ASP	C-N-CA	-5.14	114.46	122.37
1	1	185	ALA	N-CA-C	-5.14	105.86	111.82
1	4	131	ALA	O-C-N	5.14	128.76	122.75
1	3	161	MET	CA-CB-CG	-5.13	103.83	114.10
1	4	48	VAL	CB-CA-C	5.13	120.70	111.36
1	2	223	GLN	CA-C-N	-5.13	115.86	122.99
1	2	223	GLN	C-N-CA	-5.13	115.86	122.99
1	4	108	TYR	N-CA-CB	5.13	117.75	110.16
1	2	209	VAL	CB-CA-C	5.13	119.53	112.05
1	1	214	ASP	CB-CG-OD1	5.12	130.18	118.40
1	1	275	THR	O-C-N	5.12	129.06	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	43	LYS	N-CA-CB	5.12	118.22	110.28
1	2	148	SER	O-C-N	-5.12	116.06	122.35
1	2	241	LEU	CB-CA-C	5.12	118.99	110.90
1	3	48	VAL	N-CA-CB	-5.12	104.05	111.21
1	4	275	THR	CB-CA-C	-5.12	101.09	109.53
1	2	201	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	2	286	GLY	N-CA-C	5.11	118.03	110.42
1	3	67	SER	CA-C-O	-5.11	113.31	119.49
1	2	42	ASP	CA-CB-CG	-5.11	107.49	112.60
1	2	177	ILE	CA-C-N	5.11	128.47	120.75
1	2	177	ILE	C-N-CA	5.11	128.47	120.75
1	1	275	THR	CA-CB-OG1	-5.11	101.94	109.60
1	1	276	GLN	CG-CD-OE1	5.11	131.01	120.80
1	4	205	LYS	O-C-N	5.11	129.69	123.10
1	4	221	LEU	CA-CB-CG	5.11	134.18	116.30
1	2	164	GLU	CG-CD-OE2	-5.11	106.66	118.40
1	3	233	VAL	CA-C-N	5.11	132.17	123.03
1	3	233	VAL	C-N-CA	5.11	132.17	123.03
1	2	264	THR	CA-CB-CG2	5.10	119.17	110.50
1	2	308	LEU	CA-C-O	-5.10	114.94	120.81
1	3	262	ARG	N-CA-C	-5.10	106.90	113.02
1	2	269	THR	N-CA-C	-5.10	105.42	111.69
1	4	94	ILE	N-CA-CB	-5.09	104.38	111.41
1	2	168	GLY	CA-C-O	5.09	125.66	119.65
1	3	121	VAL	CA-C-O	-5.09	115.05	120.39
1	3	254	THR	CA-CB-CG2	5.09	119.15	110.50
1	4	180	GLU	CG-CD-OE1	5.09	130.10	118.40
1	3	95	VAL	CB-CA-C	5.08	118.20	110.62
1	3	136	GLY	O-C-N	5.08	127.07	122.19
1	4	87	ASP	CA-CB-CG	5.08	117.68	112.60
1	4	331	GLN	CG-CD-NE2	-5.07	108.79	116.40
1	1	289	VAL	CA-C-N	5.07	129.34	122.19
1	1	289	VAL	C-N-CA	5.07	129.34	122.19
1	4	73	ASP	O-C-N	5.07	128.51	122.27
1	4	88	SER	CA-C-N	5.07	127.58	120.28
1	4	88	SER	C-N-CA	5.07	127.58	120.28
1	4	153	ARG	CB-CA-C	-5.07	100.98	109.65
1	2	107	ALA	CA-C-O	5.07	126.10	120.63
1	1	242	ALA	CA-C-O	5.06	126.14	120.82
1	1	298	ASP	CA-C-O	-5.06	115.05	120.42
1	2	315	ILE	CA-C-O	-5.06	115.80	121.17
1	1	91	VAL	N-CA-C	-5.06	100.28	107.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	304	VAL	CA-C-O	-5.06	114.97	120.84
1	4	293	ALA	CB-CA-C	5.05	120.48	110.42
1	2	9	LEU	N-CA-C	-5.05	102.04	110.17
1	3	119	PRO	CA-C-O	-5.05	115.83	121.23
1	2	319	LEU	N-CA-C	5.05	116.64	111.03
1	1	316	LEU	CA-C-O	-5.04	115.52	120.82
1	4	203	PRO	O-C-N	-5.04	116.86	123.06
1	2	321	MET	CB-CG-SD	-5.03	97.60	112.70
1	3	271	ARG	CA-C-N	5.03	127.28	120.38
1	3	271	ARG	C-N-CA	5.03	127.28	120.38
1	3	102	THR	CA-C-O	-5.03	113.55	119.48
1	3	211	SER	O-C-N	-5.03	117.43	123.06
1	4	266	ALA	N-CA-CB	5.03	117.97	110.22
1	2	250	ILE	N-CA-CB	5.02	117.48	111.31
1	2	174	SER	CA-CB-OG	-5.01	101.07	111.10
1	3	239	LYS	CA-C-O	-5.01	115.56	120.82
1	3	172	SER	N-CA-CB	-5.01	102.21	111.53
1	1	307	ASP	CA-C-O	-5.01	113.49	119.35
1	4	187	GLY	O-C-N	5.01	126.78	121.77
1	2	227	ALA	CA-C-N	5.00	129.50	122.09
1	2	227	ALA	C-N-CA	5.00	129.50	122.09

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	332	ARG	Sidechain
1	1	35[C]	GLN	Mainchain
1	1	39[C]	VAL	Mainchain
1	2	332	ARG	Sidechain
1	3	291	ARG	Sidechain
1	3	34[C]	TYR	Mainchain
1	3	35[C]	GLN	Mainchain
1	4	153	ARG	Sidechain
1	4	262	ARG	Sidechain
1	4	35[C]	GLN	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2611	0	2621	53	5
1	2	2611	0	2624	44	0
1	3	2607	0	2618	49	0
1	4	2607	0	2618	41	0
2	1	113	0	0	1	0
2	2	87	0	0	0	0
2	3	112	0	0	2	0
2	4	106	0	0	2	5
All	All	10854	0	10481	175	5

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 9.

All (175) 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)
1:3:291:ARG:HH11	1:3:331:GLN:HE21	1.08	0.96
1:3:299:LYS:HZ1	1:3:300:ASN:HD21	1.13	0.96
1:3:299:LYS:NZ	1:3:300:ASN:HD21	1.68	0.92
1:1:291:ARG:HH11	1:1:331:GLN:HE21	1.19	0.90
1:3:256:ASN:HD21	1:3:290:LEU:H	1.26	0.84
1:4:291:ARG:HH11	1:4:331:GLN:HE21	1.24	0.82
1:4:149:ASN:ND2	1:4:151:ASP:H	1.80	0.78
1:4:149:ASN:HD22	1:4:151:ASP:H	1.28	0.78
1:3:291:ARG:NH1	1:3:331:GLN:HE21	1.83	0.76
1:3:291:ARG:HH11	1:3:331:GLN:NE2	1.83	0.74
1:1:72:ASN:HD21	1:1:314:ARG:HH22	1.35	0.73
1:4:291:ARG:NH1	1:4:331:GLN:HE21	1.85	0.73
1:3:292:ASN:HD21	1:3:298:ASP:H	1.36	0.72
1:1:304:VAL:H	1:1:331:GLN:HE22	1.39	0.70
1:2:313:ALA:O	1:2:317:VAL:HG23	1.91	0.69
1:4:48:VAL:HG13	1:4:51:LEU:HD22	1.75	0.69
1:4:319:LEU:O	1:4:322:VAL:HG22	1.92	0.69
1:3:72:ASN:HD21	1:3:314:ARG:HH22	1.41	0.68
1:4:149:ASN:HD22	1:4:150:LYS:N	1.93	0.67
1:1:254:THR:HG23	1:3:101:ASP:HB3	1.78	0.66
1:2:250:ILE:HD11	1:2:317:VAL:HG21	1.76	0.66
1:2:113:THR:HG22	1:2:319:LEU:HD11	1.80	0.64
1:1:256:ASN:HD21	1:1:290:LEU:H	1.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:82:VAL:HG13	1:1:94:ILE:HD13	1.80	0.62
1:3:11:ASN:HD22	1:3:56:ASN:HB2	1.64	0.62
1:2:193:VAL:HG12	1:2:194:GLU:HG2	1.82	0.62
1:2:278:ILE:HD13	1:2:317:VAL:HG21	1.82	0.62
1:3:292:ASN:ND2	1:3:298:ASP:H	1.99	0.61
1:4:117:ASP:HB3	1:4:209:VAL:HG11	1.83	0.61
1:4:61:GLN:HE22	1:4:64:GLN:NE2	1.98	0.60
1:3:264:THR:HB	1:3:265:PRO:HD3	1.81	0.60
1:1:250:ILE:HD11	1:1:314:ARG:HA	1.83	0.60
1:3:278:ILE:CD1	1:3:317:VAL:HG21	2.32	0.60
1:1:113:THR:HG22	1:1:319:LEU:HD11	1.84	0.59
1:1:71:THR:HG22	1:1:74:ASP:H	1.68	0.59
1:4:291:ARG:HH11	1:4:331:GLN:NE2	1.96	0.58
1:2:319:LEU:O	1:2:322:VAL:HG22	2.03	0.58
1:2:259:VAL:HG12	1:2:264:THR:HG22	1.86	0.58
1:4:18:GLY:HA2	1:4:64:GLN:NE2	2.19	0.57
1:2:48:VAL:HG22	1:2:51:LEU:HD13	1.86	0.57
1:2:276:GLN:HG3	1:2:321:MET:HE3	1.85	0.57
1:1:72:ASN:HD21	1:1:314:ARG:NH2	2.03	0.57
1:4:103:LEU:HD13	1:4:122:VAL:HG22	1.87	0.56
1:2:28[O]:ALA:HB1	1:2:47:GLY:O	2.05	0.56
1:1:9:LEU:HB3	1:1:55:ALA:HA	1.88	0.55
1:4:64:GLN:HE21	1:4:64:GLN:HA	1.71	0.55
1:4:322:VAL:HG23	1:4:323:LYS:NZ	2.22	0.55
1:1:178:LYS:HZ1	1:2:162:ASN:ND2	2.05	0.54
1:4:218:ILE:HG12	1:4:322:VAL:HG21	1.88	0.54
1:4:324:THR:HG23	1:4:330:LEU:HD13	1.89	0.54
1:4:11:ASN:HD22	1:4:56:ASN:HB2	1.73	0.54
1:2:37[O]:ALA:HB3	1:2:43:LYS:HD3	1.89	0.54
1:4:41:VAL:O	1:4:45:ILE:HG23	2.08	0.54
1:3:299:LYS:NZ	1:3:300:ASN:ND2	2.48	0.53
1:1:254:THR:HG23	1:3:101:ASP:OD2	2.08	0.53
1:4:292:ASN:HD21	1:4:298:ASP:H	1.57	0.52
1:1:72:ASN:ND2	1:1:314:ARG:HH22	2.04	0.52
1:2:113:THR:CG2	1:2:319:LEU:HD11	2.39	0.52
1:3:196:LYS:HE3	1:3:198:TYR:OH	2.09	0.52
1:3:278:ILE:HD13	1:3:317:VAL:HG21	1.91	0.52
1:4:61:GLN:NE2	1:4:64:GLN:NE2	2.58	0.52
1:3:9:LEU:HG	1:3:55:ALA:HA	1.92	0.51
1:3:137:MET:HE2	1:4:132:MET:SD	2.51	0.51
1:1:264:THR:HB	1:1:265:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:15:LEU:HD21	1:1:85:LEU:HD21	1.92	0.51
1:3:317:VAL:HG23	1:3:334:PHE:HE2	1.76	0.51
1:3:256:ASN:ND2	1:3:290:LEU:H	2.02	0.51
1:1:207:HIS:HD2	1:1:208:THR:OG1	1.94	0.51
1:1:285:GLN:NE2	1:3:285:GLN:HG3	2.26	0.51
1:1:264:THR:N	1:1:265:PRO:HD2	2.26	0.51
1:3:178:LYS:NZ	1:4:162:ASN:O	2.44	0.50
1:1:313:ALA:O	1:1:317:VAL:HG22	2.11	0.50
1:1:98:HIS:HD2	1:1:99:GLY:O	1.94	0.50
1:3:48:VAL:HG22	1:3:137:MET:HG3	1.94	0.50
1:4:278:ILE:CD1	1:4:317:VAL:HG11	2.42	0.50
1:1:278:ILE:CD1	1:1:317:VAL:HG11	2.41	0.49
1:1:178:LYS:NZ	1:2:162:ASN:ND2	2.59	0.49
1:3:82:VAL:HG12	1:3:114:LEU:HD22	1.93	0.49
1:3:314:ARG:O	1:3:318:GLU:HG3	2.11	0.49
1:3:65:ILE:HD11	1:3:70:ILE:HD12	1.93	0.49
1:3:76:LEU:HD13	1:3:221:LEU:HD22	1.94	0.49
1:2:278:ILE:HD13	1:2:317:VAL:CG2	2.43	0.49
1:2:15:LEU:HD21	1:2:85:LEU:HD11	1.95	0.49
1:2:226:ILE:HG12	1:2:250:ILE:HB	1.94	0.49
1:3:238:TYR:CE2	1:3:263:LEU:HD21	2.48	0.49
1:1:81:ARG:HH11	1:1:84:GLU:HG3	1.78	0.48
1:1:137:MET:HB2	2:1:785:HOH:O	2.13	0.48
1:1:255:GLY:HA2	1:3:173:LYS:HE2	1.95	0.48
1:1:304:VAL:H	1:1:331:GLN:NE2	2.09	0.48
1:2:248:ALA:HB2	1:2:276:GLN:HB2	1.95	0.48
1:4:166:GLN:NE2	2:4:438:HOH:O	2.46	0.48
1:1:132:MET:HE3	1:2:138:LEU:HD12	1.95	0.48
1:2:225:ASP:HB3	1:2:241:LEU:HD13	1.94	0.48
1:3:79:GLY:O	1:3:114:LEU:HD11	2.13	0.48
1:4:48:VAL:HA	1:4:137:MET:HE3	1.95	0.48
1:4:193:VAL:O	1:4:194:GLU:HB2	2.13	0.48
1:1:260:SER:HB3	1:1:263:LEU:HD13	1.95	0.47
1:4:149:ASN:HD22	1:4:149:ASN:C	2.22	0.47
1:3:114:LEU:HD23	2:3:742:HOH:O	2.15	0.47
1:4:292:ASN:HA	1:4:295:GLN:O	2.14	0.47
1:4:305:ALA:HA	1:4:334:PHE:CD2	2.49	0.47
1:1:106:THR:HG22	1:1:110:LEU:HD22	1.97	0.47
1:2:155:LYS:HD3	1:2:199:TRP:CZ3	2.48	0.47
1:4:9:LEU:HG	1:4:55:ALA:HA	1.97	0.47
1:2:223:GLN:HG2	1:2:246:ALA:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:259:VAL:CG1	1:2:264:THR:HG22	2.45	0.47
1:2:324:THR:HG21	1:2:329:GLU:HB3	1.97	0.46
1:4:48:VAL:O	1:4:51:LEU:HB2	2.15	0.46
1:3:160:THR:HA	1:3:164:GLU:O	2.16	0.46
1:3:61:GLN:NE2	1:3:63:MET:O	2.48	0.46
1:1:224:VAL:HG11	1:1:317:VAL:CG2	2.46	0.46
1:1:237:ALA:O	1:1:241:LEU:HD22	2.16	0.46
1:3:304:VAL:H	1:3:331:GLN:HE22	1.63	0.46
1:3:119:PRO:HD3	1:3:153:ARG:HG2	1.97	0.46
1:3:278:ILE:HD11	1:3:317:VAL:HG21	1.98	0.46
1:4:313:ALA:O	1:4:317:VAL:HG22	2.16	0.46
1:2:80:LYS:NZ	1:2:218:ILE:O	2.45	0.46
1:2:121:VAL:HG13	1:2:147:ALA:HB2	1.97	0.45
1:3:234:THR:HB	2:3:504:HOH:O	2.16	0.45
1:4:207:HIS:HD2	1:4:208:THR:OG1	1.99	0.45
1:4:224:VAL:HG11	1:4:317:VAL:CG2	2.46	0.45
1:3:62:VAL:HG11	1:3:78:LEU:HD23	1.99	0.45
1:4:88:SER:OG	1:4:90:ASP:HB2	2.16	0.45
1:1:224:VAL:HG11	1:1:317:VAL:HG23	1.98	0.45
1:2:47:GLY:C	1:2:49:PRO:HD3	2.42	0.45
1:2:250:ILE:HD13	1:2:278:ILE:HB	1.98	0.45
1:1:16:ALA:HA	1:1:97:THR:OG1	2.17	0.45
1:1:314:ARG:O	1:1:318:GLU:HG3	2.16	0.45
1:3:271:ARG:HA	1:3:271:ARG:HD2	1.84	0.45
1:3:237:ALA:O	1:3:241:LEU:HB2	2.17	0.45
1:1:160:THR:HA	1:1:164:GLU:O	2.17	0.44
1:1:178:LYS:NZ	1:1:178:LYS:HB3	2.32	0.44
1:1:319:LEU:O	1:1:322:VAL:HB	2.17	0.44
1:2:264:THR:N	1:2:265:PRO:CD	2.81	0.44
1:2:276:GLN:CG	1:2:321:MET:HE3	2.48	0.44
1:1:264:THR:N	1:1:265:PRO:CD	2.80	0.44
1:3:212:GLU:O	1:3:323:LYS:HE3	2.17	0.44
1:3:292:ASN:HD22	1:3:297:ASP:N	2.15	0.44
1:2:321:MET:HA	1:2:324:THR:O	2.18	0.44
1:4:278:ILE:HD13	1:4:317:VAL:HG11	1.98	0.44
1:1:113:THR:CG2	1:1:319:LEU:HD11	2.48	0.43
1:1:223:GLN:NE2	1:1:225:ASP:OD2	2.50	0.43
1:1:166:GLN:HE22	1:1:184:SER:HB3	1.83	0.43
1:1:238:TYR:OH	1:1:251:HIS:HD2	2.01	0.43
1:3:226:ILE:HG12	1:3:250:ILE:HB	2.01	0.43
1:2:314:ARG:O	1:2:318:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:81:ARG:NH1	1:1:84:GLU:HG3	2.33	0.43
1:1:8:LYS:HE3	1:1:9:LEU:HG	2.00	0.43
1:1:259:VAL:HG23	1:1:263:LEU:HB3	1.99	0.43
1:2:289:VAL:HG12	1:2:304:VAL:HG22	2.01	0.43
1:2:60:GLU:OE2	1:2:81:ARG:NH1	2.52	0.42
1:2:230:TYR:CE1	1:2:233:VAL:HG13	2.54	0.42
1:3:132:MET:HG2	1:4:137:MET:SD	2.59	0.42
1:4:178:LYS:HE3	1:4:180:GLU:OE2	2.20	0.42
1:2:214:ASP:OD1	1:2:216:LYS:HB2	2.19	0.42
1:1:230:TYR:CG	1:3:226:ILE:HD12	2.55	0.42
1:2:24[O]:ALA:CB	1:2:29[O]:ALA:HB2	2.51	0.41
1:2:15:LEU:HD21	1:2:85:LEU:CD1	2.50	0.41
1:4:194:GLU:N	2:4:699:HOH:O	2.52	0.41
1:4:250:ILE:HD11	1:4:317:VAL:HG21	2.01	0.41
1:2:47:GLY:O	1:2:49:PRO:HD3	2.21	0.41
1:3:221:LEU:HA	1:3:222:PRO:HD3	1.86	0.41
1:1:137:MET:SD	1:2:132:MET:HG2	2.61	0.41
1:2:238:TYR:CE1	1:2:263:LEU:HD11	2.55	0.41
1:1:8:LYS:NZ	1:1:9:LEU:HG	2.35	0.41
1:2:115:ASN:ND2	1:2:213:PHE:O	2.54	0.40
1:3:76:LEU:HD13	1:3:221:LEU:CD2	2.49	0.40
1:1:238:TYR:CE1	1:1:263:LEU:HD21	2.56	0.40
1:2:292:ASN:HA	1:2:295:GLN:O	2.22	0.40
1:4:224:VAL:HG11	1:4:317:VAL:HG21	2.02	0.40
1:1:47:GLY:C	1:1:49:PRO:HD3	2.46	0.40
1:1:239:LYS:O	1:1:243:GLN:HG3	2.22	0.40
1:1:213:PHE:HZ	1:1:333:ILE:HD13	1.86	0.40
1:2:103:LEU:HD21	1:2:161:MET:CE	2.52	0.40
1:3:202:LEU:HA	1:3:203:PRO:HD3	1.95	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21[C]:ILE:CD1	2:4:834:HOH:O[3_645]	0.53	1.67
1:1:21[O]:ILE:CG1	2:4:834:HOH:O[3_645]	0.86	1.34
1:1:21[O]:ILE:CD1	2:4:834:HOH:O[3_645]	0.87	1.33
1:1:21[C]:ILE:CG1	2:4:834:HOH:O[3_645]	1.07	1.13
1:1:21[O]:ILE:CB	2:4:834:HOH:O[3_645]	1.73	0.47

5.3 Torsion angles

5.3.1 Protein backbone

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	1	348/337 (103%)	328 (94%)	17 (5%)	3 (1%)	14	9
1	2	348/337 (103%)	326 (94%)	19 (6%)	3 (1%)	14	9
1	3	344/337 (102%)	326 (95%)	16 (5%)	2 (1%)	21	17
1	4	344/337 (102%)	325 (94%)	14 (4%)	5 (2%)	8	4
All	All	1384/1348 (103%)	1305 (94%)	66 (5%)	13 (1%)	18	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	26[C]	ALA
1	1	26[O]	ALA
1	2	26[C]	ALA
1	2	26[O]	ALA
1	4	26[C]	ALA
1	4	26[O]	ALA
1	2	208	THR
1	3	208	THR
1	4	208	THR
1	1	208	THR
1	4	37[C]	ALA
1	4	37[O]	ALA
1	3	177	ILE

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	1	256/266 (96%)	220 (86%)	36 (14%)	3	2
1	2	256/266 (96%)	220 (86%)	36 (14%)	3	2
1	3	256/266 (96%)	227 (89%)	29 (11%)	5	3
1	4	256/266 (96%)	225 (88%)	31 (12%)	5	3
All	All	1024/1064 (96%)	892 (87%)	132 (13%)	4	2

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	LYS
1	1	44	LEU
1	1	54	LEU
1	1	57	VAL
1	1	64	GLN
1	1	71	THR
1	1	78	LEU
1	1	85	LEU
1	1	89	ASN
1	1	101	ASP
1	1	103	LEU
1	1	110	LEU
1	1	114	LEU
1	1	123	VAL
1	1	137	MET
1	1	140	LEU
1	1	159	VAL
1	1	178	LYS
1	1	193	VAL
1	1	223	GLN
1	1	241	LEU
1	1	247	LYS
1	1	254	THR
1	1	259	VAL
1	1	263	LEU
1	1	267	LEU
1	1	272	LYS
1	1	273	THR
1	1	303	VAL
1	1	304	VAL
1	1	317	VAL
1	1	319	LEU
1	1	322	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	323	LYS
1	1	330	LEU
1	1	332	ARG
1	2	9	LEU
1	2	12	VAL
1	2	44	LEU
1	2	48	VAL
1	2	51	LEU
1	2	54	LEU
1	2	62	VAL
1	2	72	ASN
1	2	75	LEU
1	2	76	LEU
1	2	103	LEU
1	2	121	VAL
1	2	130	THR
1	2	159	VAL
1	2	178	LYS
1	2	202	LEU
1	2	209	VAL
1	2	210	ASN
1	2	219	SER
1	2	221	LEU
1	2	233	VAL
1	2	243	GLN
1	2	263	LEU
1	2	264	THR
1	2	265	PRO
1	2	267	LEU
1	2	269	THR
1	2	272	LYS
1	2	278	ILE
1	2	299	LYS
1	2	304	VAL
1	2	308	LEU
1	2	319	LEU
1	2	323	LYS
1	2	325	GLN
1	2	330	LEU
1	3	51	LEU
1	3	58	ARG
1	3	64	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	76	LEU
1	3	78	LEU
1	3	85	LEU
1	3	95	VAL
1	3	121	VAL
1	3	140	LEU
1	3	150	LYS
1	3	158	LEU
1	3	179	THR
1	3	189	LEU
1	3	192	VAL
1	3	202	LEU
1	3	221	LEU
1	3	234	THR
1	3	241	LEU
1	3	263	LEU
1	3	267	LEU
1	3	270	LEU
1	3	272	LYS
1	3	289	VAL
1	3	296	PRO
1	3	299	LYS
1	3	304	VAL
1	3	317	VAL
1	3	319	LEU
1	3	322	VAL
1	4	45	ILE
1	4	48	VAL
1	4	51	LEU
1	4	53	ASP
1	4	64	GLN
1	4	75	LEU
1	4	85	LEU
1	4	95	VAL
1	4	103	LEU
1	4	114	LEU
1	4	115	ASN
1	4	122	VAL
1	4	138	LEU
1	4	140	LEU
1	4	150	LYS
1	4	159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4	180	GLU
1	4	189	LEU
1	4	192	VAL
1	4	217	GLN
1	4	244	ASN
1	4	263	LEU
1	4	267	LEU
1	4	269	THR
1	4	272	LYS
1	4	299	LYS
1	4	304	VAL
1	4	317	VAL
1	4	319	LEU
1	4	323	LYS
1	4	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	72	ASN
1	1	89	ASN
1	1	98	HIS
1	1	115	ASN
1	1	166	GLN
1	1	207	HIS
1	1	217	GLN
1	1	251	HIS
1	1	256	ASN
1	1	285	GLN
1	1	331	GLN
1	2	56	ASN
1	2	89	ASN
1	2	149	ASN
1	2	162	ASN
1	2	207	HIS
1	2	268	GLN
1	2	284	ASN
1	2	285	GLN
1	2	325	GLN
1	3	11	ASN
1	3	61	GLN
1	3	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	162	ASN
1	3	166	GLN
1	3	223	GLN
1	3	232	ASN
1	3	244	ASN
1	3	256	ASN
1	3	292	ASN
1	3	300	ASN
1	3	306	HIS
1	3	331	GLN
1	4	11	ASN
1	4	64	GLN
1	4	149	ASN
1	4	162	ASN
1	4	166	GLN
1	4	207	HIS
1	4	223	GLN
1	4	284	ASN
1	4	292	ASN
1	4	331	GLN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	4
1	2	2
1	4	2
1	3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	19:GLY	C	20[O]:THR	N	6.29
1	2	19:GLY	C	20[C]:THR	N	5.74
1	4	19:GLY	C	20[O]:THR	N	5.25
1	1	39[O]:VAL	C	40:GLY	N	4.53
1	2	39[C]:VAL	C	40:GLY	N	4.07
1	3	39[O]:VAL	C	40:GLY	N	3.15
1	1	19:GLY	C	20[C]:THR	N	1.73
1	4	35[C]:GLN	C	36[C]:ALA	N	0.96
1	3	35[C]:GLN	C	36[C]:ALA	N	0.85
1	1	39[C]:VAL	C	40:GLY	N	0.78

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	310/337 (91%)	-0.92	0 100 100	17, 27, 55, 103	0
1	2	311/337 (92%)	-0.88	1 (0%) 90 89	18, 29, 50, 73	1 (0%)
1	3	309/337 (91%)	-1.03	0 100 100	17, 25, 44, 68	0
1	4	309/337 (91%)	-0.96	1 (0%) 90 89	16, 26, 50, 92	0
All	All	1239/1348 (91%)	-0.95	2 (0%) 91 90	16, 26, 50, 103	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	28[C]	ALA	13.0
1	4	41	VAL	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.