



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 AM UTC

PDB ID : 1TME / pdb_00001tme
Title : THREE-DIMENSIONAL STRUCTURE OF THEILER VIRUS
Authors : Grant, R.A.; Filman, D.J.; Hogle, J.M.
Deposited on : 1992-01-30
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

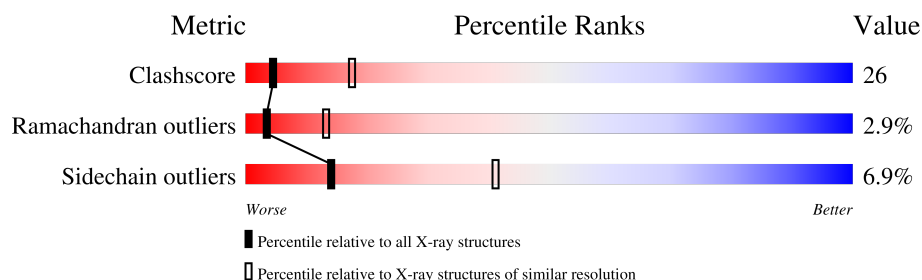
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	274	
2	2	267	
3	3	236	
4	4	71	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6280 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 THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	256	Total	C	N	O	S	0	0	0
			2005	1293	335	368	9			

- Molecule 2 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1982	1246	350	378	8			

- Molecule 3 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	230	Total	C	N	O	S	0	0	0
			1774	1139	287	336	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	202	THR	ALA	conflict	UNP P13899
3	230	VAL	ALA	conflict	UNP P13899

- Molecule 4 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	25	Total	C	N	O	0	0	0
			192	117	32	43			

- Molecule 5 is water.

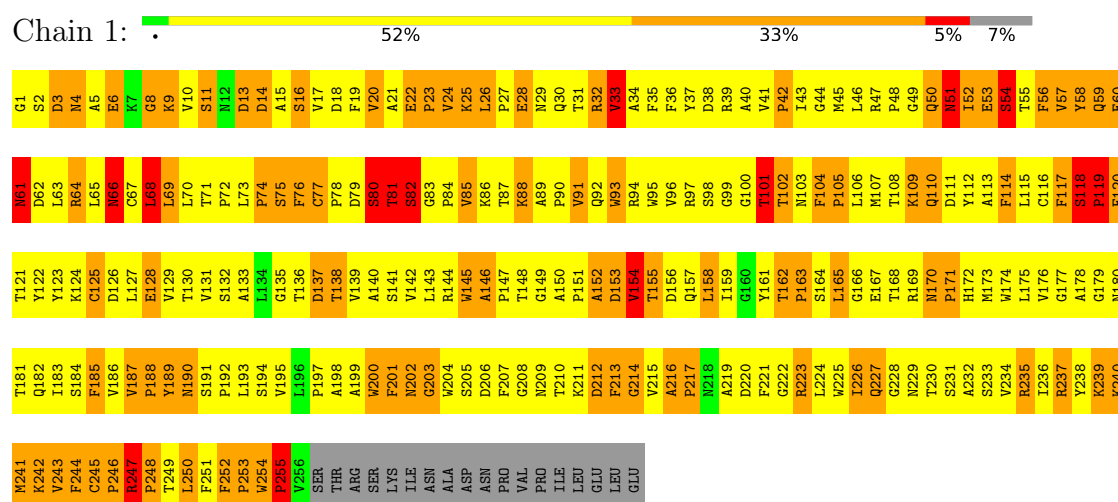
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	121	Total 121	O 121	0	0
5	2	108	Total 108	O 108	0	0
5	3	88	Total 88	O 88	0	0
5	4	10	Total 10	O 10	0	0

3 Residue-property plots

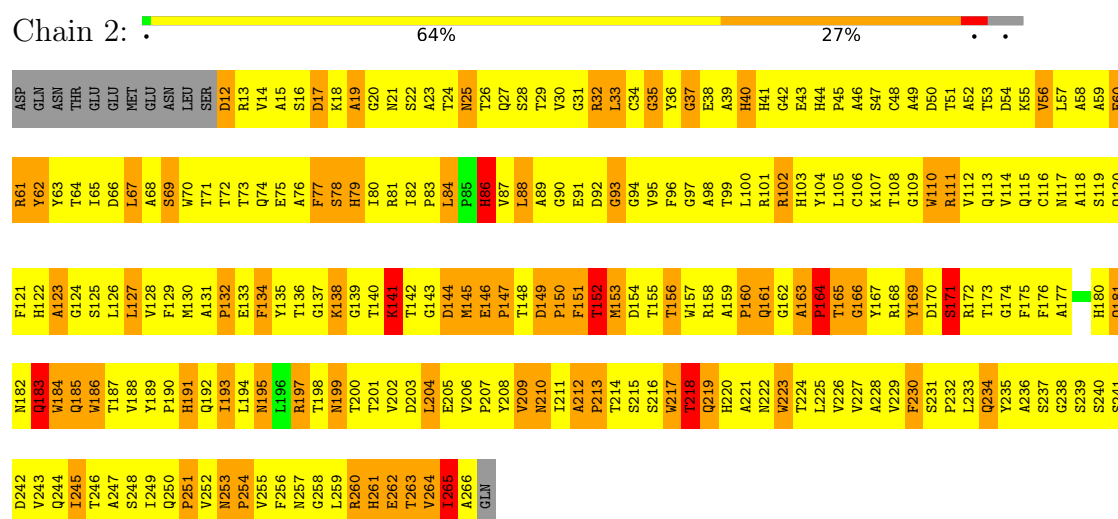
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1)

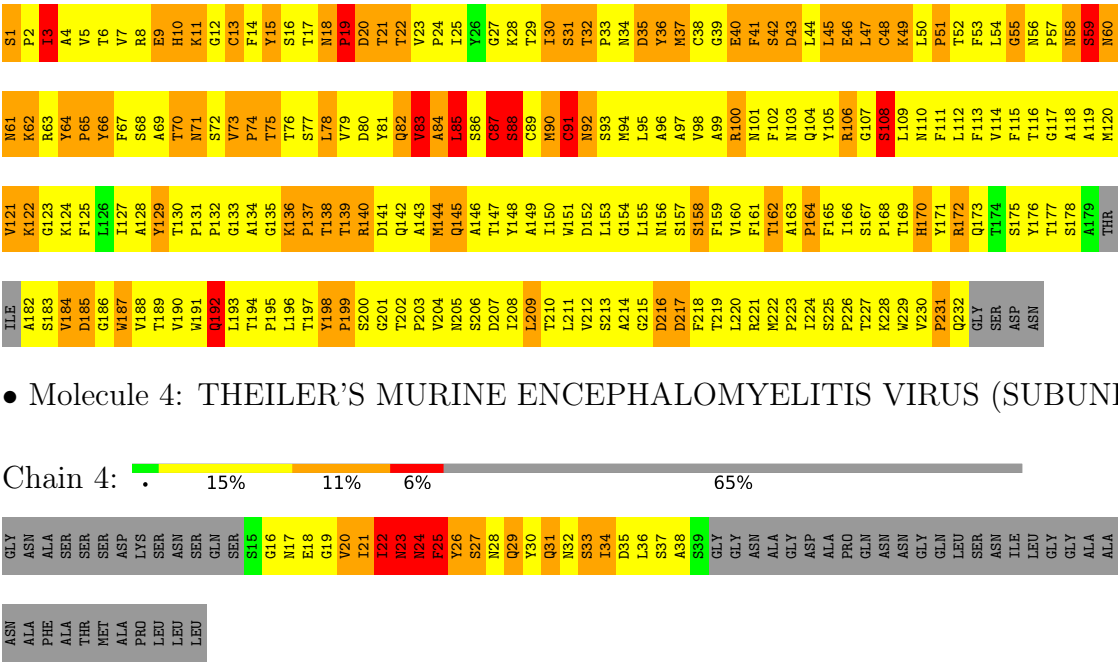


• Molecule 2: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2)



• Molecule 3: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3)





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	360.50Å 338.40Å 348.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	46.0 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	0.300 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6280	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	3.14	323/2069 (15.6%)	3.19	381/2832 (13.5%)
2	2	3.24	339/2040 (16.6%)	3.17	364/2792 (13.0%)
3	3	3.16	261/1826 (14.3%)	3.25	348/2501 (13.9%)
4	4	3.21	26/194 (13.4%)	3.06	34/262 (13.0%)
All	All	3.18	949/6129 (15.5%)	3.20	1127/8387 (13.4%)

All (949) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	131	PRO	CA-C	13.45	1.59	1.51
2	2	254	PRO	C-N	-13.16	1.17	1.33
3	3	153	LEU	C-N	-12.83	1.21	1.33
1	1	27	PRO	C-N	-12.83	1.15	1.33
1	1	90	PRO	C-N	-12.48	1.17	1.33
2	2	24	THR	C-N	-11.59	1.19	1.33
1	1	184	SER	C-N	-11.57	1.19	1.33
1	1	60	GLU	C-N	-11.40	1.19	1.33
3	3	69	ALA	C-N	-11.09	1.20	1.33
3	3	215	GLY	C-N	-10.77	1.20	1.33
1	1	226	ILE	C-N	-10.66	1.20	1.33
2	2	146	GLU	C-N	-10.50	1.20	1.33
1	1	126	ASP	C-N	-10.44	1.19	1.33
3	3	130	THR	C-N	-10.30	1.24	1.33
4	4	35	ASP	C-N	-10.29	1.20	1.33
3	3	79	VAL	C-N	-10.22	1.20	1.33
2	2	175	PHE	C-N	-10.13	1.21	1.33
2	2	78	SER	C-N	-10.02	1.20	1.33
2	2	106	CYS	C-N	-9.90	1.20	1.33
2	2	55	LYS	C-N	-9.82	1.24	1.33
2	2	160	PRO	C-N	-9.79	1.19	1.33
3	3	24	PRO	C-N	-9.67	1.22	1.34
1	1	251	PHE	C-N	-9.36	1.20	1.33
1	1	216	ALA	C-N	-9.20	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	172	ARG	C-N	-9.18	1.20	1.33
3	3	81	TYR	C-N	-9.18	1.20	1.33
2	2	190	PRO	C-N	-9.17	1.21	1.33
3	3	212	VAL	C-N	-9.12	1.22	1.33
2	2	246	THR	C-N	-9.03	1.22	1.33
1	1	162	THR	C-N	-8.96	1.24	1.33
2	2	147	PRO	C-N	-8.89	1.20	1.33
1	1	23	PRO	C-N	-8.83	1.22	1.33
2	2	173	THR	C-N	-8.81	1.21	1.33
3	3	182	ALA	N-CA	8.79	1.62	1.46
1	1	1	GLY	N-CA	8.78	1.59	1.45
4	4	33	SER	C-N	-8.74	1.23	1.33
3	3	78	LEU	C-N	-8.69	1.23	1.33
2	2	82	ILE	N-CA	8.68	1.52	1.46
2	2	202	VAL	C-N	-8.68	1.22	1.33
3	3	109	LEU	C-N	-8.67	1.19	1.33
2	2	209	VAL	C-N	-8.67	1.21	1.33
1	1	56	PHE	C-N	-8.58	1.22	1.33
3	3	137	PRO	C-N	-8.58	1.21	1.33
1	1	75	SER	C-N	-8.54	1.23	1.33
3	3	105	TYR	C-N	-8.50	1.22	1.33
2	2	16	SER	C-N	-8.47	1.22	1.33
1	1	42	PRO	C-N	-8.44	1.22	1.33
1	1	187	VAL	C-N	-8.43	1.22	1.33
2	2	251	PRO	C-N	-8.42	1.25	1.33
1	1	124	LYS	C-N	-8.39	1.22	1.33
1	1	185	PHE	C-N	-8.35	1.22	1.33
4	4	26	TYR	C-N	-8.35	1.22	1.33
4	4	27	SER	C-N	-8.35	1.23	1.33
1	1	123	TYR	C-N	-8.33	1.23	1.33
1	1	247	ARG	N-CA	8.33	1.53	1.46
3	3	68	SER	C-N	-8.31	1.22	1.33
3	3	67	PHE	C-N	-8.30	1.22	1.33
2	2	261	HIS	C-N	-8.27	1.21	1.33
3	3	1	SER	N-CA	8.26	1.61	1.46
2	2	132	PRO	C-N	-8.23	1.22	1.33
2	2	18	LYS	C-N	-8.22	1.22	1.33
1	1	145	TRP	C-N	-8.18	1.22	1.33
1	1	122	TYR	C-N	-8.17	1.23	1.33
2	2	191	HIS	C-N	-8.12	1.22	1.33
2	2	109	GLY	N-CA	8.10	1.52	1.44
2	2	236	ALA	C-N	-8.10	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	157	GLN	C-N	-8.09	1.22	1.33
1	1	175	LEU	C-N	-8.09	1.25	1.33
2	2	53	THR	C-N	-8.09	1.23	1.33
2	2	108	THR	C-N	-8.09	1.24	1.33
3	3	196	LEU	C-N	-8.07	1.22	1.33
2	2	204	LEU	C-N	-8.03	1.23	1.33
2	2	117	ASN	C-N	-8.02	1.22	1.33
3	3	146	ALA	N-CA	7.94	1.54	1.46
2	2	163	ALA	CA-C	7.92	1.60	1.52
1	1	47	ARG	C-N	-7.92	1.24	1.33
2	2	207	PRO	C-N	-7.90	1.22	1.33
2	2	227	VAL	C-N	-7.88	1.22	1.33
1	1	246	PRO	C-N	-7.88	1.23	1.33
2	2	210	ASN	C-N	-7.86	1.25	1.34
3	3	199	PRO	N-CA	7.82	1.54	1.46
1	1	135	GLY	N-CA	7.82	1.52	1.44
1	1	20	VAL	C-N	-7.78	1.26	1.33
4	4	23	ASN	C-N	-7.77	1.23	1.33
1	1	139	VAL	C-N	-7.76	1.21	1.33
2	2	192	GLN	C-N	-7.73	1.22	1.33
1	1	58	TYR	C-N	-7.72	1.23	1.33
1	1	118	SER	N-CA	7.69	1.54	1.46
1	1	183	ILE	C-N	-7.69	1.21	1.33
3	3	223	PRO	C-N	-7.67	1.22	1.33
2	2	231	SER	C-N	-7.63	1.23	1.33
2	2	234	GLN	C-N	-7.62	1.24	1.33
3	3	57	PRO	C-N	-7.57	1.22	1.33
2	2	22	SER	C-N	-7.55	1.23	1.33
3	3	60	ASN	C-O	-7.54	1.14	1.24
2	2	134	PHE	N-CA	7.53	1.55	1.46
1	1	100	GLY	N-CA	7.52	1.52	1.45
3	3	59	SER	N-CA	7.52	1.54	1.46
2	2	78	SER	CA-C	7.52	1.62	1.52
1	1	225	TRP	C-N	-7.51	1.23	1.33
1	1	44	GLY	C-N	-7.46	1.24	1.33
2	2	213	PRO	C-N	-7.45	1.23	1.33
3	3	226	PRO	C-N	-7.45	1.22	1.33
3	3	192	GLN	C-N	-7.45	1.23	1.33
1	1	146	ALA	C-N	-7.45	1.23	1.33
3	3	38	CYS	C-N	-7.45	1.23	1.33
3	3	125	PHE	C-N	-7.43	1.22	1.33
2	2	13	ARG	N-CA	7.42	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	35	PHE	N-CA	7.41	1.55	1.46
2	2	44	HIS	C-N	-7.41	1.26	1.33
1	1	162	THR	N-CA	7.40	1.53	1.45
1	1	200	TRP	C-N	-7.39	1.24	1.33
2	2	111	ARG	C-N	-7.39	1.23	1.33
1	1	113	ALA	N-CA	7.36	1.54	1.46
3	3	51	PRO	C-N	-7.35	1.23	1.33
2	2	124	GLY	C-N	-7.35	1.24	1.33
2	2	163	ALA	N-CA	7.35	1.54	1.46
1	1	78	PRO	C-N	-7.33	1.23	1.33
1	1	34	ALA	N-CA	7.31	1.54	1.46
3	3	86	SER	N-CA	7.31	1.55	1.46
1	1	14	ASP	N-CA	7.29	1.55	1.45
3	3	200	SER	C-N	-7.27	1.23	1.33
1	1	236	ILE	C-N	-7.26	1.24	1.33
2	2	118	ALA	C-N	-7.26	1.24	1.33
2	2	168	ARG	CA-C	7.23	1.62	1.52
3	3	154	GLY	C-N	-7.22	1.25	1.33
3	3	199	PRO	C-N	-7.22	1.24	1.33
3	3	52	THR	C-N	-7.21	1.23	1.33
3	3	76	THR	N-CA	7.21	1.54	1.45
2	2	109	GLY	C-N	-7.16	1.22	1.33
3	3	229	TRP	C-N	-7.15	1.25	1.33
3	3	74	PRO	C-N	-7.14	1.23	1.33
1	1	2	SER	N-CA	7.13	1.54	1.46
1	1	109	LYS	C-N	-7.13	1.23	1.33
2	2	96	PHE	N-CA	7.13	1.54	1.46
2	2	233	LEU	C-N	-7.13	1.23	1.33
2	2	223	TRP	C-N	-7.12	1.23	1.33
2	2	122	HIS	C-N	-7.10	1.23	1.33
3	3	97	ALA	N-CA	7.10	1.54	1.46
3	3	2	PRO	C-N	-7.09	1.25	1.33
2	2	76	ALA	C-N	-7.09	1.23	1.33
3	3	134	ALA	N-CA	7.08	1.54	1.46
1	1	194	SER	N-CA	7.08	1.55	1.46
2	2	162	GLY	N-CA	7.07	1.55	1.45
1	1	80	SER	N-CA	7.06	1.54	1.46
1	1	72	PRO	C-O	-7.05	1.15	1.24
2	2	81	ARG	C-N	-7.05	1.26	1.33
4	4	28	ASN	C-N	-7.04	1.24	1.33
2	2	201	THR	C-N	-7.04	1.23	1.33
3	3	56	ASN	C-N	-7.04	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	227	GLN	N-CA	7.03	1.54	1.46
2	2	159	ALA	C-N	-7.03	1.24	1.33
2	2	230	PHE	N-CA	7.03	1.54	1.46
3	3	164	PRO	C-N	-7.02	1.24	1.33
2	2	69	SER	C-N	-7.01	1.23	1.33
1	1	114	PHE	N-CA	7.00	1.55	1.46
1	1	71	THR	C-N	-6.99	1.25	1.33
2	2	265	ILE	CA-C	6.97	1.60	1.52
2	2	259	LEU	C-N	-6.97	1.24	1.33
1	1	83	GLY	N-CA	6.96	1.54	1.44
2	2	229	VAL	C-N	-6.95	1.25	1.33
3	3	96	ALA	N-CA	6.95	1.54	1.46
3	3	220	LEU	C-N	-6.94	1.24	1.33
2	2	98	ALA	N-CA	6.94	1.54	1.46
3	3	102	PHE	C-N	-6.92	1.24	1.34
1	1	142	VAL	C-N	-6.92	1.24	1.33
1	1	36	PHE	N-CA	6.90	1.54	1.46
4	4	38	ALA	N-CA	6.88	1.55	1.46
2	2	137	GLY	CA-C	6.88	1.58	1.52
2	2	177	ALA	N-CA	6.87	1.53	1.45
3	3	158	SER	C-N	-6.87	1.24	1.33
2	2	212	ALA	CA-C	6.86	1.59	1.52
3	3	14	PHE	N-CA	6.86	1.54	1.46
1	1	11	SER	C-N	-6.85	1.25	1.33
1	1	14	ASP	C-N	-6.83	1.24	1.33
2	2	142	THR	N-CA	6.83	1.54	1.46
3	3	87	CYS	N-CA	6.82	1.54	1.46
3	3	194	THR	C-N	-6.82	1.24	1.33
1	1	231	SER	C-N	-6.80	1.23	1.33
3	3	143	ALA	N-CA	6.80	1.54	1.46
2	2	216	SER	CA-C	6.79	1.61	1.53
2	2	120	GLN	N-CA	6.78	1.55	1.46
2	2	216	SER	N-CA	6.77	1.54	1.46
2	2	231	SER	CA-C	6.76	1.59	1.52
2	2	43	GLU	C-N	-6.75	1.22	1.33
1	1	43	ILE	N-CA	6.75	1.53	1.46
2	2	74	GLN	C-N	-6.75	1.23	1.33
4	4	25	PHE	N-CA	6.74	1.54	1.46
3	3	102	PHE	N-CA	6.73	1.54	1.46
1	1	28	GLU	C-N	-6.72	1.24	1.33
3	3	200	SER	CA-C	6.69	1.62	1.53
2	2	107	LYS	C-N	-6.69	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	77	CYS	CA-C	6.68	1.61	1.52
3	3	113	PHE	C-N	-6.68	1.24	1.33
2	2	220	HIS	C-N	-6.68	1.25	1.33
3	3	135	GLY	CA-C	6.68	1.59	1.52
3	3	84	ALA	N-CA	6.68	1.54	1.46
2	2	99	THR	N-CA	6.66	1.54	1.46
3	3	83	VAL	C-N	-6.66	1.24	1.33
1	1	155	THR	N-CA	6.66	1.54	1.45
1	1	40	ALA	C-N	-6.65	1.25	1.33
3	3	192	GLN	CA-C	6.64	1.61	1.52
2	2	137	GLY	N-CA	6.64	1.52	1.45
1	1	46	LEU	C-N	-6.64	1.25	1.33
2	2	244	GLN	C-N	-6.63	1.24	1.33
3	3	119	ALA	N-CA	6.62	1.54	1.46
3	3	117	GLY	C-N	-6.62	1.24	1.33
1	1	120	PHE	N-CA	6.61	1.54	1.45
1	1	48	PRO	C-N	-6.60	1.25	1.34
1	1	74	PRO	C-N	-6.60	1.25	1.33
2	2	58	ALA	N-CA	6.60	1.54	1.46
1	1	198	ALA	N-CA	6.59	1.54	1.46
1	1	102	THR	C-N	-6.59	1.25	1.33
2	2	168	ARG	C-N	-6.59	1.24	1.33
3	3	197	THR	N-CA	6.59	1.53	1.45
2	2	115	GLN	C-N	-6.59	1.24	1.33
2	2	46	ALA	N-CA	6.59	1.54	1.46
2	2	136	THR	N-CA	6.59	1.54	1.46
2	2	97	GLY	CA-C	6.58	1.59	1.52
1	1	102	THR	N-CA	6.58	1.54	1.45
1	1	221	PHE	N-CA	6.58	1.54	1.46
2	2	128	VAL	C-N	-6.58	1.24	1.33
3	3	40	GLU	C-N	-6.58	1.24	1.33
4	4	26	TYR	CA-C	6.57	1.60	1.52
3	3	30	ILE	C-N	-6.57	1.24	1.33
3	3	93	SER	N-CA	6.57	1.54	1.45
3	3	29	THR	C-N	-6.57	1.25	1.33
2	2	249	ILE	C-N	-6.57	1.26	1.33
2	2	245	ILE	C-N	-6.56	1.24	1.33
3	3	89	CYS	N-CA	6.56	1.54	1.46
1	1	15	ALA	N-CA	6.55	1.54	1.46
3	3	211	LEU	C-N	-6.55	1.23	1.33
2	2	152	THR	N-CA	6.54	1.53	1.46
4	4	18	GLU	N-CA	6.54	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	33	SER	CA-C	6.53	1.60	1.52
1	1	101	THR	N-CA	6.53	1.53	1.46
2	2	110	TRP	C-N	-6.52	1.24	1.33
2	2	119	SER	N-CA	6.50	1.53	1.46
2	2	162	GLY	CA-C	6.50	1.59	1.52
2	2	43	GLU	CA-C	6.50	1.60	1.52
2	2	161	GLN	CA-C	6.49	1.60	1.52
2	2	13	ARG	C-O	-6.49	1.15	1.24
2	2	123	ALA	C-N	-6.48	1.24	1.33
1	1	79	ASP	C-N	-6.47	1.25	1.33
3	3	62	LYS	N-CA	6.47	1.54	1.45
1	1	96	VAL	C-N	-6.46	1.25	1.33
3	3	216	ASP	N-CA	6.45	1.54	1.46
3	3	214	ALA	C-N	-6.45	1.24	1.33
2	2	89	ALA	N-CA	6.45	1.54	1.46
2	2	155	THR	N-CA	6.42	1.54	1.46
1	1	203	GLY	CA-C	6.42	1.58	1.51
2	2	239	SER	N-CA	6.41	1.53	1.46
3	3	22	THR	C-N	-6.41	1.25	1.33
2	2	82	ILE	CA-C	6.40	1.58	1.53
2	2	118	ALA	N-CA	6.40	1.54	1.46
2	2	214	THR	N-CA	6.39	1.54	1.45
2	2	237	SER	C-N	-6.39	1.24	1.33
2	2	219	GLN	N-CA	6.39	1.53	1.46
2	2	151	PHE	N-CA	6.39	1.53	1.46
3	3	31	SER	N-CA	6.38	1.54	1.46
1	1	213	PHE	N-CA	6.37	1.54	1.46
2	2	25	ASN	C-N	-6.37	1.24	1.33
3	3	124	LYS	C-N	-6.37	1.24	1.33
1	1	116	CYS	N-CA	6.37	1.54	1.46
2	2	260	ARG	N-CA	6.37	1.53	1.46
2	2	61	ARG	C-N	-6.35	1.24	1.33
3	3	186	GLY	N-CA	6.35	1.51	1.45
2	2	168	ARG	N-CA	6.34	1.54	1.45
1	1	237	ARG	N-CA	6.34	1.54	1.46
3	3	121	VAL	C-N	-6.34	1.24	1.33
3	3	106	ARG	N-CA	6.33	1.53	1.46
1	1	89	ALA	CA-C	6.32	1.59	1.53
1	1	70	LEU	C-N	-6.32	1.25	1.33
1	1	81	THR	N-CA	6.32	1.54	1.46
3	3	163	ALA	CA-C	6.32	1.60	1.52
2	2	174	GLY	N-CA	6.29	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	16	GLY	N-CA	6.29	1.52	1.45
2	2	219	GLN	C-N	-6.29	1.25	1.33
2	2	103	HIS	C-N	-6.29	1.25	1.33
3	3	61	ASN	C-N	-6.29	1.24	1.33
3	3	146	ALA	C-N	-6.29	1.24	1.33
4	4	22	ILE	N-CA	6.28	1.54	1.46
2	2	146	GLU	CA-C	6.28	1.60	1.52
3	3	148	TYR	C-N	-6.28	1.24	1.33
1	1	125	CYS	C-N	-6.28	1.24	1.33
2	2	250	GLN	CA-C	6.28	1.57	1.52
3	3	231	PRO	N-CA	6.28	1.55	1.47
1	1	209	ASN	C-N	-6.28	1.24	1.33
1	1	99	GLY	CA-C	6.27	1.59	1.51
2	2	139	GLY	N-CA	6.27	1.52	1.45
3	3	145	GLN	N-CA	6.27	1.54	1.46
1	1	216	ALA	CA-C	6.27	1.60	1.52
3	3	38	CYS	CA-C	6.26	1.61	1.53
1	1	227	GLN	C-N	-6.26	1.21	1.33
2	2	205	GLU	C-N	-6.26	1.26	1.33
2	2	200	THR	N-CA	6.25	1.54	1.46
1	1	89	ALA	C-N	-6.25	1.25	1.33
1	1	152	ALA	N-CA	6.25	1.54	1.46
2	2	212	ALA	N-CA	6.25	1.53	1.45
2	2	72	THR	N-CA	6.25	1.54	1.46
2	2	30	VAL	N-CA	6.24	1.52	1.46
1	1	154	VAL	N-CA	6.24	1.54	1.46
2	2	76	ALA	CA-C	6.23	1.60	1.52
2	2	240	SER	N-CA	6.23	1.54	1.46
3	3	16	SER	N-CA	6.23	1.54	1.46
2	2	53	THR	CA-C	6.22	1.60	1.52
2	2	90	GLY	C-N	-6.22	1.25	1.33
2	2	19	ALA	N-CA	6.22	1.54	1.46
2	2	59	ALA	N-CA	6.22	1.54	1.46
1	1	182	GLN	C-N	-6.21	1.25	1.33
2	2	237	SER	N-CA	6.20	1.54	1.46
2	2	49	ALA	N-CA	6.20	1.54	1.46
3	3	77	SER	N-CA	6.20	1.53	1.45
2	2	45	PRO	CA-C	6.19	1.58	1.52
2	2	175	PHE	N-CA	6.19	1.54	1.46
3	3	131	PRO	N-CA	6.19	1.54	1.46
1	1	82	SER	N-CA	6.18	1.53	1.46
2	2	226	VAL	C-N	-6.18	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	208	TYR	C-N	-6.18	1.24	1.33
3	3	46	GLU	N-CA	6.17	1.53	1.46
3	3	139	THR	N-CA	6.17	1.53	1.46
3	3	185	ASP	N-CA	6.17	1.53	1.46
3	3	41	PHE	N-CA	6.16	1.53	1.45
1	1	66	ASN	C-O	-6.16	1.16	1.24
2	2	47	SER	N-CA	6.16	1.54	1.46
1	1	94	ARG	C-N	-6.16	1.25	1.33
1	1	214	GLY	N-CA	6.16	1.53	1.45
3	3	217	ASP	N-CA	6.16	1.54	1.46
1	1	118	SER	CA-C	6.16	1.59	1.53
2	2	37	GLY	CA-C	6.15	1.57	1.51
2	2	48	CYS	N-CA	6.15	1.53	1.46
2	2	131	ALA	C-N	-6.15	1.25	1.33
3	3	171	TYR	C-N	-6.15	1.24	1.33
2	2	218	THR	N-CA	6.14	1.54	1.46
3	3	209	LEU	C-N	-6.14	1.24	1.33
1	1	52	ILE	CA-C	6.14	1.59	1.52
3	3	226	PRO	N-CA	6.14	1.54	1.47
2	2	121	PHE	N-CA	6.14	1.54	1.46
1	1	14	ASP	CA-C	6.13	1.60	1.52
2	2	221	ALA	CA-C	6.13	1.60	1.53
3	3	75	THR	N-CA	6.12	1.54	1.46
3	3	4	ALA	C-N	-6.12	1.24	1.33
1	1	94	ARG	N-CA	6.11	1.54	1.46
3	3	214	ALA	N-CA	6.11	1.53	1.46
1	1	224	LEU	C-N	-6.11	1.24	1.33
4	4	36	LEU	C-N	-6.10	1.24	1.33
1	1	138	THR	CA-C	6.09	1.60	1.52
3	3	142	GLN	N-CA	6.09	1.53	1.46
2	2	265	ILE	C-O	-6.08	1.17	1.24
2	2	238	GLY	N-CA	6.08	1.54	1.45
1	1	206	ASP	N-CA	6.07	1.53	1.46
1	1	189	TYR	CA-C	6.07	1.60	1.52
2	2	171	SER	N-CA	6.07	1.53	1.46
1	1	93	TRP	C-N	-6.06	1.25	1.33
1	1	247	ARG	C-N	-6.06	1.25	1.33
2	2	151	PHE	C-N	-6.06	1.25	1.33
2	2	132	PRO	N-CA	6.05	1.54	1.47
2	2	221	ALA	N-CA	6.05	1.54	1.46
2	2	82	ILE	C-N	-6.05	1.25	1.33
3	3	214	ALA	CA-C	6.05	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	27	GLN	N-CA	6.05	1.53	1.46
3	3	135	GLY	C-N	-6.04	1.23	1.33
2	2	150	PRO	C-O	-6.04	1.16	1.24
3	3	125	PHE	N-CA	6.04	1.53	1.45
2	2	176	PHE	N-CA	6.04	1.53	1.46
2	2	40	HIS	C-N	-6.03	1.24	1.33
2	2	256	PHE	C-N	-6.03	1.25	1.33
3	3	4	ALA	N-CA	6.03	1.53	1.46
2	2	123	ALA	N-CA	6.03	1.53	1.45
1	1	168	THR	N-CA	6.02	1.53	1.46
1	1	85	VAL	N-CA	6.02	1.53	1.46
3	3	183	SER	N-CA	6.02	1.53	1.46
1	1	91	VAL	C-N	-6.01	1.24	1.33
2	2	97	GLY	N-CA	6.01	1.53	1.45
1	1	219	ALA	N-CA	6.00	1.53	1.46
2	2	114	VAL	C-N	-6.00	1.25	1.33
2	2	102	ARG	N-CA	6.00	1.53	1.46
1	1	172	HIS	C-N	-5.99	1.24	1.33
3	3	109	LEU	CA-C	5.99	1.60	1.52
3	3	163	ALA	C-N	-5.99	1.25	1.33
2	2	78	SER	N-CA	5.99	1.53	1.46
2	2	80	ILE	C-N	-5.99	1.25	1.33
1	1	169	ARG	N-CA	5.98	1.53	1.46
3	3	93	SER	CA-C	5.98	1.60	1.52
1	1	96	VAL	N-CA	5.98	1.53	1.46
3	3	227	THR	CA-C	5.98	1.61	1.52
2	2	76	ALA	N-CA	5.97	1.53	1.46
3	3	85	LEU	N-CA	5.97	1.53	1.46
1	1	56	PHE	N-CA	5.97	1.53	1.46
1	1	42	PRO	N-CA	5.97	1.54	1.47
1	1	157	GLN	CA-C	5.97	1.60	1.52
1	1	178	ALA	N-CA	5.97	1.53	1.46
3	3	46	GLU	C-O	-5.96	1.17	1.24
1	1	31	THR	C-N	-5.96	1.25	1.33
1	1	163	PRO	CA-C	5.96	1.58	1.52
3	3	118	ALA	N-CA	5.96	1.53	1.46
1	1	5	ALA	N-CA	5.95	1.53	1.46
3	3	17	THR	N-CA	5.95	1.53	1.46
2	2	148	THR	N-CA	5.95	1.53	1.46
3	3	99	ALA	N-CA	5.95	1.53	1.46
1	1	84	PRO	C-N	-5.94	1.25	1.33
2	2	167	TYR	C-N	-5.94	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	28	LYS	C-N	-5.94	1.25	1.33
3	3	50	LEU	C-N	-5.94	1.26	1.33
3	3	154	GLY	N-CA	5.93	1.52	1.45
3	3	111	PHE	N-CA	5.92	1.53	1.46
2	2	60	GLU	C-N	-5.92	1.25	1.33
1	1	159	ILE	N-CA	5.92	1.53	1.46
3	3	169	THR	N-CA	5.92	1.52	1.45
3	3	156	ASN	C-N	-5.92	1.26	1.34
1	1	203	GLY	N-CA	5.91	1.51	1.45
1	1	41	VAL	N-CA	5.91	1.53	1.46
2	2	14	VAL	C-N	-5.91	1.25	1.33
1	1	86	LYS	C-N	-5.91	1.24	1.33
3	3	72	SER	C-N	-5.91	1.26	1.33
2	2	214	THR	C-N	-5.91	1.25	1.33
3	3	91	CYS	N-CA	5.91	1.53	1.46
2	2	228	ALA	C-N	-5.90	1.24	1.33
3	3	62	LYS	C-N	-5.90	1.25	1.33
3	3	13	CYS	C-N	-5.89	1.25	1.33
3	3	41	PHE	C-N	-5.89	1.25	1.33
3	3	170	HIS	N-CA	5.88	1.53	1.46
2	2	265	ILE	N-CA	5.88	1.53	1.46
1	1	35	PHE	C-O	-5.87	1.17	1.24
1	1	44	GLY	CA-C	5.87	1.58	1.51
3	3	54	LEU	C-N	-5.87	1.25	1.33
1	1	201	PHE	N-CA	5.86	1.54	1.46
1	1	233	SER	N-CA	5.86	1.53	1.46
2	2	16	SER	N-CA	5.86	1.53	1.46
3	3	60	ASN	CA-C	5.86	1.60	1.52
1	1	147	PRO	N-CA	5.86	1.54	1.47
3	3	83	VAL	N-CA	5.86	1.53	1.46
2	2	87	VAL	N-CA	5.86	1.53	1.46
2	2	66	ASP	C-N	-5.85	1.26	1.33
3	3	137	PRO	N-CA	5.84	1.54	1.47
3	3	146	ALA	CA-C	5.83	1.60	1.53
2	2	63	TYR	CA-C	5.83	1.60	1.52
2	2	185	GLN	N-CA	5.83	1.53	1.46
1	1	148	THR	CA-C	5.83	1.59	1.52
1	1	205	SER	N-CA	5.83	1.53	1.46
2	2	127	LEU	C-N	-5.83	1.25	1.33
2	2	248	SER	N-CA	5.83	1.53	1.46
2	2	64	THR	N-CA	5.83	1.53	1.46
1	1	113	ALA	CA-C	5.82	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	105	PRO	C-N	-5.82	1.25	1.33
2	2	135	TYR	C-N	-5.82	1.26	1.33
1	1	195	VAL	N-CA	5.82	1.52	1.46
1	1	254	TRP	CA-C	5.82	1.59	1.52
3	3	115	PHE	N-CA	5.82	1.53	1.46
3	3	213	SER	N-CA	5.82	1.53	1.46
3	3	113	PHE	N-CA	5.81	1.53	1.46
3	3	132	PRO	C-N	-5.81	1.25	1.33
3	3	201	GLY	C-N	-5.81	1.25	1.33
1	1	164	SER	N-CA	5.81	1.53	1.46
3	3	188	VAL	C-N	-5.80	1.25	1.33
1	1	242	LYS	C-N	-5.80	1.24	1.33
2	2	113	GLN	CA-C	5.79	1.59	1.52
2	2	152	THR	C-N	-5.79	1.25	1.33
3	3	24	PRO	N-CA	5.78	1.54	1.47
3	3	117	GLY	N-CA	5.78	1.53	1.45
2	2	73	THR	N-CA	5.78	1.53	1.46
2	2	192	GLN	CA-C	5.78	1.59	1.52
1	1	166	GLY	N-CA	5.77	1.53	1.45
3	3	138	THR	N-CA	5.77	1.53	1.46
2	2	28	SER	N-CA	5.77	1.53	1.46
3	3	177	THR	N-CA	5.77	1.53	1.46
2	2	156	THR	N-CA	5.76	1.52	1.46
2	2	184	TRP	N-CA	5.76	1.53	1.46
3	3	65	PRO	N-CA	5.76	1.54	1.47
2	2	29	THR	C-N	-5.76	1.26	1.33
1	1	122	TYR	CA-C	5.76	1.59	1.52
1	1	11	SER	CA-C	5.76	1.59	1.52
1	1	251	PHE	N-CA	5.75	1.53	1.46
1	1	233	SER	C-N	-5.75	1.25	1.33
1	1	39	ARG	N-CA	5.74	1.53	1.46
1	1	64	ARG	CA-C	5.74	1.59	1.52
2	2	239	SER	CA-C	5.74	1.60	1.52
4	4	22	ILE	C-N	-5.74	1.25	1.33
1	1	247	ARG	CA-C	5.74	1.57	1.52
1	1	18	ASP	N-CA	5.74	1.53	1.46
3	3	59	SER	CA-C	5.74	1.60	1.52
1	1	49	GLY	N-CA	5.74	1.53	1.45
1	1	39	ARG	C-N	-5.73	1.25	1.33
1	1	178	ALA	CA-C	5.73	1.60	1.52
2	2	31	GLY	N-CA	5.73	1.50	1.45
2	2	180	HIS	C-N	-5.73	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	159	ALA	CA-C	5.73	1.59	1.53
2	2	160	PRO	N-CA	5.73	1.53	1.47
2	2	213	PRO	N-CA	5.73	1.54	1.47
1	1	110	GLN	C-N	-5.72	1.26	1.33
2	2	26	THR	N-CA	5.72	1.53	1.46
3	3	173	GLN	N-CA	5.72	1.53	1.46
2	2	241	SER	N-CA	5.72	1.53	1.46
2	2	62	TYR	CA-C	5.72	1.59	1.52
2	2	255	VAL	C-N	-5.72	1.25	1.33
1	1	174	TRP	N-CA	5.71	1.53	1.46
2	2	83	PRO	N-CA	5.71	1.53	1.47
2	2	20	GLY	C-N	-5.71	1.25	1.33
1	1	237	ARG	CA-C	5.71	1.59	1.52
2	2	176	PHE	C-N	-5.71	1.25	1.33
3	3	83	VAL	CA-C	5.71	1.59	1.52
3	3	89	CYS	CA-C	5.71	1.60	1.52
3	3	19	PRO	C-N	-5.71	1.26	1.33
1	1	53	GLU	N-CA	5.70	1.53	1.46
1	1	217	PRO	N-CA	5.70	1.54	1.47
3	3	166	ILE	C-N	-5.70	1.26	1.33
1	1	21	ALA	CA-C	5.70	1.59	1.53
1	1	26	LEU	C-N	-5.69	1.26	1.33
4	4	27	SER	CA-C	5.69	1.59	1.52
1	1	140	ALA	N-CA	5.68	1.54	1.47
1	1	195	VAL	CA-C	5.68	1.59	1.52
1	1	104	PHE	N-CA	5.67	1.54	1.45
1	1	144	ARG	C-N	-5.67	1.25	1.33
2	2	90	GLY	CA-C	5.67	1.58	1.51
1	1	31	THR	N-CA	5.66	1.52	1.46
1	1	71	THR	CA-C	5.66	1.59	1.52
1	1	132	SER	N-CA	5.66	1.53	1.46
3	3	223	PRO	CA-C	5.66	1.58	1.52
2	2	161	GLN	N-CA	5.66	1.53	1.46
4	4	21	ILE	N-CA	5.66	1.53	1.46
1	1	104	PHE	C-N	-5.65	1.23	1.34
1	1	102	THR	CA-C	5.65	1.60	1.53
1	1	39	ARG	CA-C	5.65	1.59	1.52
2	2	125	SER	N-CA	5.64	1.52	1.46
1	1	163	PRO	C-N	-5.64	1.26	1.33
1	1	210	THR	N-CA	5.64	1.53	1.45
2	2	77	PHE	N-CA	5.64	1.53	1.46
3	3	119	ALA	CA-C	5.63	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	16	SER	N-CA	5.63	1.53	1.46
2	2	139	GLY	CA-C	5.63	1.57	1.51
1	1	143	LEU	C-N	-5.63	1.25	1.33
4	4	18	GLU	CA-C	5.62	1.59	1.52
3	3	21	THR	C-N	-5.62	1.24	1.33
3	3	163	ALA	N-CA	5.62	1.54	1.46
3	3	110	ASN	C-N	-5.62	1.25	1.33
2	2	92	ASP	N-CA	5.61	1.53	1.46
2	2	111	ARG	CA-C	5.61	1.59	1.52
1	1	48	PRO	CA-C	5.61	1.58	1.52
3	3	166	ILE	N-CA	5.61	1.52	1.46
3	3	94	MET	N-CA	5.61	1.53	1.46
3	3	135	GLY	N-CA	5.61	1.52	1.45
1	1	27	PRO	CA-C	5.61	1.59	1.52
1	1	254	TRP	C-N	-5.61	1.20	1.33
3	3	106	ARG	C-N	-5.61	1.24	1.33
2	2	75	GLU	N-CA	5.60	1.52	1.45
1	1	133	ALA	N-CA	5.60	1.53	1.46
1	1	128	GLU	CA-C	5.60	1.59	1.52
3	3	67	PHE	N-CA	5.60	1.53	1.45
1	1	207	PHE	N-CA	5.60	1.53	1.46
4	4	24	ASN	CA-C	5.59	1.57	1.52
1	1	3	ASP	N-CA	5.59	1.54	1.46
2	2	39	ALA	N-CA	5.59	1.52	1.45
1	1	128	GLU	C-N	-5.58	1.25	1.33
2	2	137	GLY	C-N	-5.58	1.26	1.33
1	1	199	ALA	N-CA	5.58	1.53	1.46
2	2	131	ALA	CA-C	5.58	1.57	1.52
3	3	178	SER	N-CA	5.58	1.53	1.46
2	2	107	LYS	N-CA	5.58	1.52	1.46
3	3	7	VAL	N-CA	5.58	1.52	1.46
4	4	31	GLN	N-CA	5.58	1.53	1.46
1	1	72	PRO	N-CA	5.58	1.54	1.47
3	3	176	TYR	CA-C	5.58	1.60	1.52
3	3	95	LEU	N-CA	5.57	1.52	1.46
3	3	72	SER	N-CA	5.57	1.52	1.46
2	2	165	THR	N-CA	5.57	1.53	1.46
1	1	255	PRO	N-CA	5.56	1.54	1.47
1	1	38	ASP	N-CA	5.56	1.53	1.46
3	3	116	THR	N-CA	5.56	1.53	1.46
3	3	101	ASN	N-CA	5.56	1.53	1.46
1	1	27	PRO	N-CA	5.56	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	33	SER	N-CA	5.56	1.53	1.46
1	1	49	GLY	CA-C	5.55	1.59	1.51
3	3	131	PRO	C-N	-5.55	1.20	1.33
1	1	148	THR	N-CA	5.55	1.53	1.46
3	3	4	ALA	CA-C	5.55	1.60	1.52
3	3	200	SER	N-CA	5.55	1.53	1.45
3	3	194	THR	N-CA	5.54	1.54	1.45
1	1	87	THR	N-CA	5.54	1.53	1.46
2	2	147	PRO	N-CA	5.54	1.53	1.47
2	2	242	ASP	C-N	-5.54	1.26	1.33
1	1	151	PRO	CA-C	5.54	1.59	1.52
3	3	111	PHE	C-N	-5.54	1.25	1.33
3	3	38	CYS	N-CA	5.54	1.53	1.45
2	2	263	THR	C-N	-5.53	1.26	1.33
2	2	101	ARG	N-CA	5.53	1.53	1.46
2	2	122	HIS	CA-C	5.53	1.59	1.52
3	3	161	PHE	N-CA	5.53	1.52	1.46
1	1	231	SER	N-CA	5.53	1.53	1.45
3	3	196	LEU	CA-C	5.52	1.60	1.52
2	2	19	ALA	CA-C	5.52	1.58	1.53
3	3	31	SER	CA-C	5.52	1.59	1.52
1	1	8	GLY	N-CA	5.52	1.52	1.45
2	2	38	GLU	N-CA	5.52	1.53	1.46
2	2	197	ARG	N-CA	5.52	1.53	1.46
3	3	6	THR	N-CA	5.52	1.53	1.46
3	3	219	THR	C-N	-5.52	1.25	1.33
1	1	113	ALA	C-O	-5.52	1.17	1.24
1	1	249	THR	N-CA	5.52	1.52	1.45
2	2	207	PRO	N-CA	5.52	1.54	1.47
2	2	17	ASP	N-CA	5.51	1.52	1.46
3	3	52	THR	N-CA	5.51	1.53	1.45
2	2	63	TYR	C-N	-5.51	1.25	1.33
3	3	69	ALA	N-CA	5.51	1.53	1.45
3	3	195	PRO	N-CA	5.51	1.53	1.47
2	2	150	PRO	N-CA	5.51	1.54	1.47
3	3	40	GLU	CA-C	5.51	1.59	1.52
2	2	157	TRP	C-N	-5.51	1.25	1.33
1	1	151	PRO	N-CA	5.50	1.53	1.47
3	3	160	VAL	C-N	-5.50	1.25	1.33
3	3	141	ASP	N-CA	5.50	1.52	1.46
1	1	204	TRP	N-CA	5.50	1.53	1.45
2	2	237	SER	CA-C	5.50	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	86	SER	CA-C	5.49	1.60	1.52
3	3	203	PRO	N-CA	5.49	1.54	1.47
3	3	168	PRO	C-O	-5.49	1.17	1.24
3	3	227	THR	N-CA	5.49	1.53	1.46
2	2	160	PRO	CA-C	5.49	1.59	1.52
3	3	96	ALA	CA-C	5.49	1.59	1.52
1	1	150	ALA	C-N	-5.48	1.26	1.33
2	2	71	THR	N-CA	5.48	1.52	1.45
3	3	188	VAL	CA-C	5.48	1.59	1.52
1	1	109	LYS	N-CA	5.48	1.52	1.45
1	1	243	VAL	C-N	-5.48	1.26	1.33
2	2	119	SER	C-N	-5.48	1.26	1.33
2	2	203	ASP	C-N	-5.48	1.25	1.33
3	3	98	VAL	N-CA	5.48	1.53	1.46
4	4	37	SER	N-CA	5.48	1.53	1.46
3	3	98	VAL	CA-C	5.47	1.59	1.52
2	2	14	VAL	CA-C	5.47	1.59	1.52
3	3	140	ARG	N-CA	5.47	1.53	1.46
2	2	240	SER	CA-C	5.47	1.60	1.52
1	1	220	ASP	N-CA	5.47	1.52	1.45
1	1	188	PRO	N-CA	5.47	1.53	1.47
2	2	189	TYR	CA-C	5.47	1.60	1.53
1	1	111	ASP	CA-C	5.46	1.59	1.53
1	1	23	PRO	CA-C	5.46	1.58	1.52
2	2	81	ARG	N-CA	5.46	1.52	1.46
2	2	253	ASN	N-CA	5.46	1.51	1.46
3	3	97	ALA	CA-C	5.46	1.59	1.52
4	4	24	ASN	N-CA	5.46	1.52	1.46
3	3	100	ARG	N-CA	5.45	1.53	1.46
1	1	40	ALA	N-CA	5.45	1.52	1.46
1	1	246	PRO	N-CA	5.45	1.53	1.47
2	2	193	ILE	C-N	-5.45	1.26	1.33
2	2	217	TRP	N-CA	5.45	1.53	1.46
1	1	93	TRP	N-CA	5.45	1.52	1.45
2	2	41	HIS	N-CA	5.45	1.53	1.46
2	2	46	ALA	CA-C	5.45	1.60	1.52
1	1	228	GLY	N-CA	5.44	1.52	1.44
2	2	198	THR	N-CA	5.44	1.53	1.46
1	1	146	ALA	CA-C	5.44	1.58	1.52
2	2	123	ALA	CA-C	5.44	1.59	1.52
1	1	80	SER	CA-C	5.43	1.59	1.52
2	2	251	PRO	N-CA	5.43	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	154	ASP	N-CA	5.43	1.53	1.46
1	1	60	GLU	CA-C	5.43	1.59	1.52
1	1	90	PRO	CA-C	5.43	1.58	1.52
2	2	154	ASP	C-N	-5.43	1.25	1.33
1	1	131	VAL	N-CA	5.42	1.53	1.46
1	1	197	PRO	C-N	-5.42	1.26	1.34
4	4	29	GLN	N-CA	5.42	1.53	1.46
1	1	185	PHE	N-CA	5.42	1.52	1.46
3	3	207	ASP	C-N	-5.42	1.25	1.33
1	1	79	ASP	N-CA	5.42	1.52	1.45
2	2	211	ILE	N-CA	5.42	1.53	1.46
1	1	126	ASP	CA-C	5.41	1.59	1.52
2	2	225	LEU	C-N	-5.41	1.26	1.33
1	1	21	ALA	N-CA	5.41	1.53	1.46
2	2	65	ILE	C-N	-5.41	1.25	1.33
3	3	122	LYS	C-N	-5.40	1.25	1.33
3	3	133	GLY	N-CA	5.40	1.53	1.45
2	2	115	GLN	N-CA	5.40	1.52	1.46
3	3	30	ILE	CA-C	5.40	1.58	1.52
3	3	19	PRO	N-CA	5.40	1.54	1.47
3	3	201	GLY	N-CA	5.40	1.53	1.45
1	1	136	THR	C-N	-5.39	1.26	1.33
2	2	98	ALA	CA-C	5.39	1.59	1.52
1	1	119	PRO	C-N	-5.39	1.26	1.33
1	1	214	GLY	CA-C	5.39	1.59	1.51
2	2	208	TYR	CA-C	5.39	1.59	1.52
3	3	194	THR	CA-C	5.39	1.59	1.52
1	1	67	CYS	N-CA	5.39	1.52	1.46
3	3	82	GLN	N-CA	5.39	1.53	1.46
1	1	45	MET	C-N	-5.38	1.26	1.33
2	2	70	TRP	N-CA	5.38	1.52	1.46
3	3	78	LEU	N-CA	5.38	1.52	1.46
3	3	21	THR	N-CA	5.38	1.52	1.45
1	1	153	ASP	N-CA	5.38	1.53	1.46
3	3	12	GLY	N-CA	5.38	1.53	1.45
2	2	257	ASN	C-N	-5.37	1.25	1.33
2	2	15	ALA	N-CA	5.37	1.52	1.45
2	2	177	ALA	C-N	-5.37	1.26	1.33
1	1	64	ARG	N-CA	5.37	1.53	1.46
1	1	220	ASP	C-N	-5.36	1.26	1.33
2	2	100	LEU	N-CA	5.36	1.52	1.46
2	2	155	THR	C-N	-5.36	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	147	THR	N-CA	5.36	1.52	1.46
2	2	236	ALA	CA-C	5.36	1.59	1.52
4	4	22	ILE	CA-C	5.36	1.59	1.52
2	2	62	TYR	C-N	-5.36	1.25	1.33
1	1	219	ALA	CA-C	5.35	1.59	1.52
2	2	252	VAL	N-CA	5.35	1.52	1.46
1	1	140	ALA	CA-C	5.35	1.59	1.53
1	1	150	ALA	N-CA	5.35	1.53	1.45
2	2	15	ALA	C-N	-5.35	1.25	1.33
1	1	233	SER	CA-C	5.35	1.59	1.52
1	1	180	ASN	N-CA	5.34	1.53	1.46
1	1	74	PRO	N-CA	5.34	1.53	1.47
1	1	24	VAL	C-N	-5.34	1.26	1.33
1	1	119	PRO	N-CA	5.34	1.54	1.47
3	3	65	PRO	C-O	-5.34	1.17	1.24
2	2	109	GLY	CA-C	5.34	1.59	1.52
1	1	76	PHE	N-CA	5.34	1.53	1.46
1	1	107	MET	N-CA	5.34	1.52	1.46
2	2	121	PHE	C-O	-5.34	1.16	1.23
2	2	246	THR	N-CA	5.33	1.52	1.45
3	3	193	LEU	N-CA	5.33	1.52	1.46
1	1	42	PRO	CA-C	5.33	1.58	1.52
3	3	10	HIS	C-N	-5.33	1.26	1.33
3	3	143	ALA	CA-C	5.33	1.59	1.52
1	1	20	VAL	CA-C	5.33	1.59	1.52
1	1	244	PHE	N-CA	5.33	1.52	1.45
2	2	119	SER	CA-C	5.33	1.59	1.52
3	3	76	THR	C-N	-5.33	1.26	1.33
1	1	144	ARG	CA-C	5.33	1.59	1.52
3	3	149	ALA	C-N	-5.33	1.24	1.33
3	3	112	LEU	C-N	-5.32	1.26	1.33
3	3	228	LYS	C-N	-5.32	1.26	1.33
1	1	91	VAL	N-CA	5.32	1.52	1.46
1	1	17	VAL	N-CA	5.32	1.52	1.46
1	1	164	SER	CA-C	5.32	1.59	1.52
3	3	171	TYR	CA-C	5.32	1.59	1.52
2	2	162	GLY	C-N	-5.31	1.27	1.33
1	1	184	SER	N-CA	5.31	1.52	1.46
1	1	170	ASN	CA-C	5.31	1.59	1.53
3	3	218	PHE	N-CA	5.31	1.53	1.46
3	3	132	PRO	N-CA	5.31	1.54	1.47
3	3	221	ARG	N-CA	5.31	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	51	ASN	C-N	-5.30	1.27	1.34
2	2	94	GLY	N-CA	5.30	1.53	1.45
3	3	159	PHE	N-CA	5.30	1.52	1.46
2	2	172	ARG	N-CA	5.30	1.52	1.45
1	1	155	THR	C-N	-5.29	1.26	1.33
1	1	167	GLU	C-N	-5.29	1.26	1.33
1	1	186	VAL	C-N	-5.29	1.27	1.33
2	2	214	THR	CA-C	5.29	1.59	1.52
3	3	147	THR	C-N	-5.29	1.27	1.33
1	1	96	VAL	CA-C	5.29	1.58	1.52
2	2	69	SER	N-CA	5.29	1.53	1.46
1	1	167	GLU	N-CA	5.29	1.53	1.46
1	1	192	PRO	N-CA	5.29	1.54	1.47
1	1	84	PRO	N-CA	5.28	1.54	1.47
1	1	98	SER	N-CA	5.28	1.53	1.46
1	1	163	PRO	N-CA	5.28	1.53	1.47
2	2	138	LYS	N-CA	5.28	1.52	1.46
3	3	2	PRO	N-CA	5.28	1.53	1.47
1	1	98	SER	CA-C	5.28	1.59	1.52
1	1	47	ARG	CA-C	5.28	1.58	1.52
1	1	97	ARG	N-CA	5.27	1.52	1.46
1	1	19	PHE	N-CA	5.27	1.52	1.45
3	3	168	PRO	N-CA	5.27	1.54	1.47
1	1	121	THR	N-CA	5.27	1.52	1.46
1	1	150	ALA	CA-C	5.27	1.59	1.53
1	1	55	THR	C-N	-5.27	1.26	1.33
3	3	48	CYS	N-CA	5.27	1.52	1.46
1	1	111	ASP	N-CA	5.27	1.53	1.46
2	2	20	GLY	CA-C	5.27	1.59	1.52
1	1	66	ASN	N-CA	5.26	1.52	1.46
2	2	45	PRO	N-CA	5.26	1.53	1.47
1	1	121	THR	C-N	-5.26	1.25	1.33
1	1	130	THR	C-N	-5.26	1.25	1.33
3	3	212	VAL	N-CA	5.26	1.52	1.46
1	1	228	GLY	C-N	-5.25	1.26	1.33
1	1	188	PRO	C-N	-5.25	1.26	1.33
2	2	88	LEU	N-CA	5.25	1.52	1.46
3	3	199	PRO	CA-C	5.24	1.58	1.53
2	2	95	VAL	N-CA	5.24	1.52	1.46
3	3	9	GLU	N-CA	5.24	1.52	1.46
3	3	25	ILE	C-N	-5.24	1.26	1.33
1	1	77	CYS	N-CA	5.24	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	42	SER	N-CA	5.24	1.52	1.46
2	2	187	THR	N-CA	5.23	1.53	1.46
3	3	42	SER	C-N	-5.23	1.26	1.33
1	1	83	GLY	CA-C	5.23	1.59	1.51
3	3	225	SER	C-N	-5.23	1.27	1.33
2	2	56	VAL	CA-C	5.23	1.57	1.53
2	2	142	THR	CA-C	5.23	1.59	1.52
3	3	118	ALA	CA-C	5.23	1.59	1.52
1	1	44	GLY	N-CA	5.22	1.52	1.45
1	1	89	ALA	N-CA	5.22	1.52	1.45
1	1	108	THR	C-N	-5.22	1.25	1.33
2	2	261	HIS	CA-C	5.22	1.59	1.52
1	1	249	THR	C-N	-5.22	1.26	1.33
2	2	105	LEU	C-N	-5.22	1.26	1.33
3	3	3	ILE	CA-C	5.22	1.58	1.52
3	3	225	SER	CA-C	5.22	1.59	1.52
2	2	164	PRO	C-N	-5.21	1.26	1.33
2	2	190	PRO	N-CA	5.21	1.53	1.47
1	1	147	PRO	C-N	-5.21	1.26	1.33
2	2	66	ASP	N-CA	5.21	1.52	1.46
1	1	107	MET	C-O	-5.21	1.18	1.24
1	1	138	THR	N-CA	5.21	1.52	1.46
2	2	246	THR	CA-C	5.21	1.59	1.52
1	1	34	ALA	CA-C	5.21	1.59	1.52
1	1	204	TRP	C-N	-5.20	1.25	1.33
3	3	159	PHE	C-N	-5.20	1.26	1.33
1	1	252	PHE	N-CA	5.20	1.54	1.46
3	3	33	PRO	N-CA	5.20	1.53	1.47
2	2	248	SER	CA-C	5.19	1.59	1.52
2	2	253	ASN	C-O	-5.19	1.21	1.23
2	2	12	ASP	N-CA	5.19	1.56	1.46
1	1	154	VAL	C-O	-5.19	1.17	1.24
1	1	158	LEU	N-CA	5.19	1.52	1.46
2	2	104	TYR	N-CA	5.19	1.52	1.46
3	3	142	GLN	C-O	-5.18	1.18	1.24
1	1	28	GLU	N-CA	5.18	1.52	1.46
1	1	81	THR	CA-C	5.18	1.59	1.52
3	3	33	PRO	CA-C	5.17	1.58	1.52
1	1	99	GLY	N-CA	5.17	1.53	1.45
1	1	161	TYR	C-N	-5.17	1.25	1.33
3	3	226	PRO	CA-C	5.17	1.58	1.52
2	2	22	SER	CA-C	5.16	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	231	SER	N-CA	5.16	1.53	1.46
2	2	186	TRP	NE1-CE2	-5.16	1.31	1.37
2	2	58	ALA	CA-C	5.16	1.59	1.52
1	1	136	THR	N-CA	5.16	1.52	1.46
1	1	179	GLY	N-CA	5.16	1.53	1.44
3	3	47	LEU	C-O	-5.16	1.18	1.24
1	1	157	GLN	N-CA	5.15	1.52	1.46
2	2	69	SER	CA-C	5.15	1.59	1.52
3	3	230	VAL	CA-C	5.15	1.58	1.52
1	1	130	THR	CA-C	5.15	1.58	1.52
2	2	20	GLY	N-CA	5.15	1.53	1.45
3	3	22	THR	N-CA	5.14	1.53	1.46
1	1	17	VAL	CA-C	5.14	1.58	1.52
3	3	64	TYR	CA-C	5.14	1.57	1.52
3	3	72	SER	CA-C	5.14	1.58	1.52
3	3	84	ALA	CA-C	5.14	1.59	1.52
2	2	50	ASP	N-CA	5.14	1.52	1.46
2	2	53	THR	N-CA	5.14	1.52	1.46
2	2	37	GLY	C-N	-5.14	1.27	1.33
3	3	215	GLY	N-CA	5.14	1.52	1.45
1	1	207	PHE	C-O	-5.13	1.17	1.24
3	3	32	THR	CA-C	5.13	1.59	1.52
2	2	232	PRO	N-CA	5.13	1.53	1.47
3	3	172	ARG	N-CA	5.13	1.52	1.46
1	1	43	ILE	C-N	-5.13	1.27	1.33
2	2	70	TRP	C-N	-5.13	1.26	1.33
1	1	174	TRP	NE1-CE2	-5.13	1.31	1.37
3	3	104	GLN	CA-C	5.13	1.58	1.52
2	2	228	ALA	N-CA	5.13	1.52	1.46
2	2	254	PRO	N-CA	5.13	1.53	1.47
2	2	110	TRP	NE1-CE2	-5.12	1.31	1.37
2	2	112	VAL	C-N	-5.12	1.26	1.33
3	3	104	GLN	N-CA	5.12	1.52	1.45
1	1	126	ASP	N-CA	5.12	1.51	1.45
1	1	59	GLN	C-N	-5.12	1.25	1.33
1	1	222	GLY	CA-C	5.12	1.57	1.52
2	2	61	ARG	N-CA	5.12	1.52	1.46
2	2	244	GLN	CA-C	5.12	1.60	1.53
3	3	151	TRP	NE1-CE2	-5.12	1.31	1.37
1	1	197	PRO	N-CA	5.12	1.53	1.47
3	3	106	ARG	CA-C	5.12	1.58	1.52
1	1	145	TRP	NE1-CE2	-5.12	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	200	TRP	NE1-CE2	-5.12	1.31	1.37
1	1	93	TRP	NE1-CE2	-5.11	1.31	1.37
2	2	54	ASP	N-CA	5.11	1.52	1.46
2	2	217	TRP	NE1-CE2	-5.11	1.31	1.37
2	2	70	TRP	NE1-CE2	-5.10	1.31	1.37
2	2	141	LYS	CA-C	5.10	1.59	1.52
2	2	183	GLN	N-CA	5.10	1.52	1.46
3	3	66	TYR	C-N	-5.10	1.26	1.33
2	2	259	LEU	N-CA	5.10	1.52	1.46
2	2	223	TRP	NE1-CE2	-5.10	1.31	1.37
2	2	125	SER	C-N	-5.09	1.26	1.33
2	2	256	PHE	N-CA	5.09	1.52	1.46
3	3	229	TRP	NE1-CE2	-5.09	1.31	1.37
2	2	64	THR	C-N	-5.09	1.27	1.33
3	3	76	THR	CA-C	5.09	1.60	1.53
3	3	187	TRP	NE1-CE2	-5.09	1.31	1.37
1	1	204	TRP	NE1-CE2	-5.09	1.31	1.37
1	1	179	GLY	CA-C	5.09	1.58	1.51
2	2	133	GLU	CA-C	5.09	1.60	1.53
2	2	157	TRP	NE1-CE2	-5.09	1.31	1.37
2	2	247	ALA	N-CA	5.09	1.52	1.46
1	1	15	ALA	CA-C	5.09	1.59	1.52
1	1	92	GLN	C-N	-5.09	1.25	1.33
1	1	225	TRP	NE1-CE2	-5.09	1.31	1.37
2	2	24	THR	CA-C	5.09	1.60	1.53
1	1	187	VAL	CA-C	5.09	1.58	1.52
2	2	51	THR	C-N	-5.09	1.26	1.33
3	3	165	PHE	N-CA	5.08	1.53	1.46
1	1	198	ALA	CA-C	5.08	1.59	1.52
2	2	172	ARG	CA-C	5.08	1.59	1.53
3	3	206	SER	C-N	-5.08	1.26	1.33
3	3	191	TRP	NE1-CE2	-5.08	1.31	1.37
2	2	245	ILE	CA-C	5.08	1.59	1.52
2	2	247	ALA	C-N	-5.08	1.25	1.33
3	3	54	LEU	N-CA	5.07	1.52	1.46
3	3	207	ASP	N-CA	5.07	1.52	1.46
1	1	23	PRO	N-CA	5.07	1.53	1.47
1	1	95	TRP	NE1-CE2	-5.07	1.31	1.37
2	2	84	LEU	N-CA	5.07	1.53	1.45
2	2	118	ALA	CA-C	5.07	1.59	1.52
1	1	62	ASP	CA-C	5.07	1.59	1.53
1	1	203	GLY	C-N	-5.07	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	254	TRP	NE1-CE2	-5.06	1.31	1.37
2	2	184	TRP	NE1-CE2	-5.06	1.31	1.37
1	1	115	LEU	N-CA	5.06	1.52	1.46
1	1	181	THR	C-N	-5.06	1.25	1.33
2	2	202	VAL	CA-C	5.06	1.58	1.52
1	1	30	GLN	N-CA	5.06	1.52	1.46
1	1	240	LYS	C-O	-5.06	1.17	1.23
1	1	110	GLN	N-CA	5.06	1.52	1.46
2	2	197	ARG	CA-C	5.06	1.59	1.52
1	1	255	PRO	CA-C	5.05	1.59	1.52
2	2	205	GLU	CA-C	5.05	1.58	1.52
4	4	30	TYR	CA-C	5.05	1.59	1.52
2	2	253	ASN	CA-C	5.04	1.56	1.53
1	1	231	SER	CA-C	5.04	1.59	1.52
2	2	199	ASN	N-CA	5.04	1.52	1.45
1	1	128	GLU	N-CA	5.04	1.52	1.46
2	2	227	VAL	CA-C	5.04	1.59	1.52
1	1	78	PRO	N-CA	5.03	1.53	1.47
2	2	169	TYR	CA-C	5.03	1.59	1.52
3	3	223	PRO	N-CA	5.03	1.53	1.47
2	2	16	SER	CA-C	5.03	1.58	1.52
2	2	103	HIS	N-CA	5.03	1.52	1.46
2	2	190	PRO	CA-C	5.03	1.59	1.52
1	1	241	MET	C-N	-5.03	1.26	1.33
2	2	143	GLY	N-CA	5.03	1.52	1.45
2	2	146	GLU	N-CA	5.03	1.53	1.46
3	3	88	SER	N-CA	5.03	1.52	1.46
1	1	252	PHE	C-N	-5.02	1.22	1.33
2	2	132	PRO	CA-C	5.02	1.59	1.52
2	2	154	ASP	CA-C	5.02	1.59	1.52
1	1	90	PRO	N-CA	5.02	1.53	1.47
1	1	248	PRO	N-CA	5.02	1.53	1.47
2	2	93	GLY	N-CA	5.02	1.53	1.45
2	2	164	PRO	N-CA	5.02	1.53	1.47
3	3	190	VAL	C-N	-5.02	1.26	1.33
2	2	22	SER	N-CA	5.01	1.52	1.45
1	1	152	ALA	CA-C	5.01	1.59	1.52
2	2	129	PHE	C-N	-5.01	1.26	1.33
2	2	261	HIS	N-CA	5.01	1.52	1.46
1	1	235	ARG	CA-C	5.01	1.58	1.52
2	2	240	SER	C-N	-5.01	1.26	1.33
3	3	202	THR	CA-C	5.01	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	136	LYS	N-CA	5.00	1.53	1.45

All (1127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	131	PRO	O-C-N	21.14	131.04	121.31
3	3	218	PHE	N-CA-C	13.11	129.51	110.24
3	3	53	PHE	N-CA-C	12.46	128.64	109.96
3	3	131	PRO	CA-C-O	-11.78	112.42	120.90
3	3	167	SER	O-C-N	11.75	130.07	121.85
3	3	23	VAL	N-CA-C	11.68	120.40	108.95
2	2	151	PHE	N-CA-C	11.43	125.73	112.93
2	2	129	PHE	N-CA-C	11.38	126.09	109.14
1	1	26	LEU	O-C-N	11.29	132.27	121.66
3	3	202	THR	O-C-N	11.21	131.37	121.39
1	1	170	ASN	O-C-N	11.05	133.81	121.43
3	3	88	SER	N-CA-C	11.04	125.27	111.69
2	2	212	ALA	O-C-N	10.99	129.68	121.88
2	2	262	GLU	N-CA-C	10.94	125.67	109.59
2	2	163	ALA	O-C-N	10.93	131.75	121.04
1	1	13	ASP	N-CA-C	10.69	123.55	110.41
1	1	247	ARG	O-C-N	10.60	130.55	121.54
3	3	184	VAL	N-CA-C	10.51	124.15	108.80
1	1	19	PHE	N-CA-C	10.49	125.78	109.52
2	2	176	PHE	N-CA-C	10.46	124.79	108.79
1	1	36	PHE	N-CA-C	10.33	122.12	111.07
3	3	64	TYR	O-C-N	10.29	131.81	121.72
1	1	113	ALA	O-C-N	10.29	132.73	122.03
1	1	222	GLY	O-C-N	10.23	131.37	122.88
1	1	223	ARG	N-CA-C	10.20	124.17	108.96
2	2	95	VAL	O-C-N	10.20	131.76	121.87
3	3	46	GLU	O-C-N	10.17	132.90	122.12
1	1	244	PHE	N-CA-C	10.17	124.59	109.24
1	1	89	ALA	O-C-N	10.09	131.69	121.30
2	2	253	ASN	CB-CA-C	-10.05	101.26	110.71
2	2	131	ALA	O-C-N	9.88	131.40	121.72
2	2	253	ASN	O-C-N	9.87	132.66	121.32
1	1	76	PHE	O-C-N	9.86	132.28	123.41
1	1	162	THR	O-C-N	9.72	129.61	121.35
3	3	79	VAL	O-C-N	9.70	133.39	122.82
2	2	174	GLY	O-C-N	9.69	132.15	122.65
3	3	92	ASN	N-CA-C	9.62	125.29	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	120	PHE	N-CA-C	9.62	124.13	109.23
2	2	256	PHE	N-CA-C	9.61	124.90	109.24
3	3	103	ASN	N-CA-C	9.60	122.96	111.82
3	3	18	ASN	O-C-N	9.55	128.92	121.47
3	3	194	THR	O-C-N	9.52	130.81	121.57
2	2	215	SER	N-CA-C	9.48	124.85	109.40
3	3	142	GLN	O-C-N	9.43	132.27	122.09
2	2	159	ALA	O-C-N	9.37	131.93	121.43
1	1	71	THR	O-C-N	9.31	131.56	122.06
1	1	118	SER	O-C-N	9.29	129.88	121.42
1	1	185	PHE	N-CA-C	9.23	122.17	108.14
3	3	50	LEU	O-C-N	9.22	131.93	121.32
1	1	50	GLN	N-CA-C	9.14	122.77	108.79
3	3	163	ALA	O-C-N	9.13	131.82	121.32
3	3	63	ARG	N-CA-C	9.09	125.23	109.96
1	1	22	GLU	O-C-N	9.05	131.73	121.32
2	2	146	GLU	O-C-N	9.02	131.69	121.32
3	3	226	PRO	CA-C-O	-9.02	110.54	122.08
2	2	112	VAL	N-CA-C	8.99	121.42	108.48
1	1	221	PHE	N-CA-C	8.96	122.97	112.93
1	1	47	ARG	O-C-N	8.94	132.09	121.10
2	2	82	ILE	O-C-N	8.88	129.09	120.92
2	2	149	ASP	O-C-N	8.80	131.44	121.32
2	2	222	ASN	N-CA-C	8.79	121.82	111.71
1	1	216	ALA	O-C-N	8.77	130.05	121.28
2	2	189	TYR	O-C-N	8.77	132.78	121.64
3	3	56	ASN	O-C-N	8.69	128.70	121.31
3	3	61	ASN	N-CA-C	8.67	122.99	111.28
1	1	211	LYS	N-CA-C	8.67	123.79	109.06
1	1	4	ASN	CB-CA-C	-8.66	100.35	111.70
3	3	115	PHE	N-CA-C	8.65	121.61	109.15
4	4	26	TYR	O-C-N	8.64	133.07	123.22
3	3	73	VAL	O-C-N	8.64	130.95	121.10
2	2	43	GLU	O-C-N	8.61	133.46	122.87
2	2	250	GLN	O-C-N	8.58	130.92	121.23
1	1	150	ALA	O-C-N	8.56	130.95	121.53
1	1	76	PHE	N-CA-C	8.53	121.64	108.07
3	3	230	VAL	O-C-N	8.53	130.83	121.10
1	1	68	LEU	N-CA-C	8.52	122.44	109.23
3	3	199	PRO	O-C-N	8.50	132.66	123.23
2	2	37	GLY	O-C-N	8.49	129.39	122.51
1	1	229	ASN	N-CA-C	8.48	123.20	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	260	ARG	O-C-N	8.41	131.99	122.99
3	3	41	PHE	N-CA-C	8.40	122.25	109.23
3	3	141	ASP	O-C-N	8.39	130.81	122.09
3	3	175	SER	N-CA-C	8.39	123.25	109.24
1	1	104	PHE	N-CA-C	8.38	122.93	110.10
1	1	9	LYS	O-C-N	8.38	130.95	123.41
1	1	51	ASN	CB-CA-C	-8.36	93.78	110.42
2	2	38	GLU	N-CA-C	8.36	121.29	108.42
3	3	157	SER	N-CA-C	8.34	121.30	111.71
2	2	199	ASN	N-CA-C	8.30	122.02	108.99
2	2	265	ILE	CB-CA-C	-8.28	101.10	111.70
1	1	35	PHE	O-C-N	8.28	130.70	122.09
2	2	254	PRO	O-C-N	8.27	132.94	122.85
3	3	158	SER	N-CA-C	8.26	122.44	109.81
1	1	139	VAL	N-CA-C	8.25	120.43	109.21
1	1	32	ARG	O-C-N	8.24	132.62	123.22
2	2	39	ALA	N-CA-C	8.22	122.88	109.72
3	3	226	PRO	O-C-N	8.22	133.03	123.00
2	2	78	SER	CA-C-O	-8.22	112.15	121.19
1	1	146	ALA	O-C-N	8.17	130.40	122.06
1	1	56	PHE	N-CA-C	8.14	122.04	110.23
1	1	117	PHE	N-CA-C	8.13	124.52	108.18
1	1	234	VAL	N-CA-C	8.12	119.38	107.37
1	1	42	PRO	CA-C-O	-8.11	112.55	121.23
1	1	58	TYR	O-C-N	8.11	132.19	123.11
2	2	97	GLY	O-C-N	8.10	129.97	122.19
1	1	251	PHE	N-CA-C	8.09	121.65	110.24
1	1	176	VAL	N-CA-C	8.08	118.40	108.06
1	1	9	LYS	N-CA-C	8.07	120.91	108.07
3	3	198	TYR	O-C-N	8.07	130.60	121.32
3	3	159	PHE	N-CA-C	8.06	122.00	108.13
3	3	97	ALA	O-C-N	8.06	130.66	122.12
3	3	225	SER	O-C-N	8.06	131.11	121.60
1	1	29	ASN	N-CA-C	8.05	124.27	113.97
1	1	83	GLY	O-C-N	8.05	129.82	121.77
1	1	4	ASN	N-CA-C	8.04	120.59	107.32
2	2	68	ALA	N-CA-C	8.04	120.80	108.42
1	1	91	VAL	O-C-N	8.03	131.83	123.00
2	2	235	TYR	O-C-N	8.02	132.62	123.48
3	3	113	PHE	N-CA-C	7.99	121.93	109.07
3	3	32	THR	O-C-N	7.96	130.47	121.32
3	3	96	ALA	O-C-N	7.93	130.52	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	34	ALA	O-C-N	7.92	130.56	122.08
1	1	157	GLN	CB-CA-C	-7.92	99.06	110.06
1	1	137	ASP	O-C-N	7.91	132.35	123.01
1	1	191	SER	N-CA-C	7.91	119.74	109.93
3	3	140	ARG	O-C-N	7.91	131.21	122.11
3	3	128	ALA	N-CA-C	7.91	121.99	109.50
2	2	160	PRO	CA-C-O	-7.90	112.08	121.95
3	3	164	PRO	O-C-N	7.89	132.58	123.03
3	3	167	SER	N-CA-C	7.89	121.01	108.23
3	3	130	THR	O-C-N	7.87	130.09	121.12
3	3	192	GLN	O-C-N	7.85	132.68	123.02
1	1	10	VAL	O-C-N	7.85	131.89	123.02
1	1	254	TRP	O-C-N	7.84	128.47	121.18
3	3	79	VAL	CA-C-O	-7.82	113.63	121.45
1	1	103	ASN	N-CA-C	7.82	120.79	111.33
1	1	126	ASP	O-C-N	7.82	131.86	123.03
1	1	112	TYR	O-C-N	7.80	130.39	122.12
2	2	172	ARG	O-C-N	7.78	131.87	122.84
3	3	143	ALA	O-C-N	7.78	130.18	122.09
2	2	41	HIS	CA-CB-CG	-7.78	106.02	113.80
3	3	199	PRO	CA-C-O	-7.77	112.40	121.96
1	1	230	THR	N-CA-C	7.76	121.88	108.76
1	1	73	LEU	O-C-N	7.75	129.81	121.60
3	3	66	TYR	N-CA-C	7.75	118.84	108.38
3	3	37	MET	N-CA-C	7.75	121.46	110.23
1	1	188	PRO	O-C-N	7.74	132.57	123.06
3	3	45	LEU	O-C-N	7.73	130.31	122.12
2	2	191	HIS	N-CA-C	7.71	118.79	108.38
2	2	206	VAL	O-C-N	7.71	129.89	121.10
2	2	202	VAL	O-C-N	7.70	131.34	123.10
1	1	185	PHE	O-C-N	7.70	130.99	123.29
2	2	98	ALA	O-C-N	7.69	130.28	122.12
2	2	236	ALA	O-C-N	7.69	132.26	122.81
3	3	114	VAL	O-C-N	7.67	131.20	122.99
3	3	3	ILE	O-C-N	7.67	131.42	122.83
1	1	10	VAL	N-CA-C	7.67	121.63	108.90
1	1	24	VAL	CB-CA-C	-7.67	103.37	112.19
2	2	60	GLU	N-CA-C	7.67	120.52	109.71
2	2	231	SER	O-C-N	7.67	130.53	121.10
2	2	79	HIS	N-CA-C	7.66	120.38	108.96
1	1	27	PRO	CA-C-O	-7.64	112.88	121.43
2	2	162	GLY	O-C-N	7.63	129.57	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	244	GLN	O-C-N	7.63	131.49	122.94
3	3	213	SER	O-C-N	7.62	131.58	123.42
2	2	44	HIS	O-C-N	7.62	129.96	121.43
2	2	78	SER	O-C-N	7.62	132.24	122.87
1	1	129	VAL	N-CA-C	7.61	119.24	108.36
1	1	86	LYS	N-CA-C	7.61	122.00	112.87
2	2	75	GLU	O-C-N	7.60	131.65	122.84
1	1	242	LYS	O-C-N	7.58	132.61	123.36
3	3	99	ALA	O-C-N	7.58	130.16	122.12
3	3	222	MET	O-C-N	7.56	130.02	121.32
1	1	53	GLU	O-C-N	7.56	131.41	122.34
3	3	117	GLY	O-C-N	7.55	130.37	122.59
1	1	181	THR	N-CA-C	7.54	124.60	114.12
3	3	16	SER	O-C-N	7.52	130.09	122.12
1	1	213	PHE	N-CA-C	7.51	121.28	110.24
1	1	215	VAL	N-CA-C	7.51	118.49	107.37
3	3	195	PRO	O-C-N	7.51	132.32	123.01
4	4	32	ASN	O-C-N	7.51	131.98	123.27
1	1	163	PRO	O-C-N	7.50	130.98	123.03
1	1	54	SER	N-CA-C	7.50	120.48	109.69
4	4	32	ASN	N-CA-C	7.50	120.85	109.23
1	1	77	CYS	O-C-N	7.49	129.93	121.32
1	1	35	PHE	CB-CA-C	-7.49	98.83	110.81
1	1	187	VAL	O-C-N	7.48	129.62	121.10
1	1	231	SER	O-C-N	7.47	131.41	122.96
2	2	255	VAL	O-C-N	7.47	131.12	123.20
1	1	207	PHE	O-C-N	7.45	130.70	122.20
1	1	17	VAL	N-CA-C	7.43	117.40	110.42
3	3	149	ALA	O-C-N	7.42	132.31	123.33
2	2	158	ARG	O-C-N	7.41	131.67	123.22
1	1	190	ASN	N-CA-C	7.41	122.03	112.92
2	2	52	ALA	N-CA-C	7.41	120.42	110.35
3	3	217	ASP	CB-CA-C	-7.41	96.93	110.63
1	1	232	ALA	N-CA-C	7.40	121.64	109.06
2	2	243	VAL	N-CA-C	7.40	119.04	107.28
1	1	186	VAL	N-CA-C	7.39	118.45	108.11
3	3	11	LYS	N-CA-C	7.39	120.40	110.35
2	2	254	PRO	CA-C-O	-7.38	113.28	121.32
1	1	125	CYS	O-C-N	7.37	132.40	122.59
2	2	73	THR	O-C-N	7.37	129.94	122.12
4	4	22	ILE	CB-CA-C	-7.37	99.21	111.29
3	3	195	PRO	CA-C-O	-7.35	113.03	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	55	THR	O-C-N	7.33	132.04	123.02
1	1	57	VAL	O-C-N	7.33	130.99	123.07
2	2	15	ALA	N-CA-C	7.32	120.58	109.23
3	3	146	ALA	O-C-N	7.32	131.37	121.78
1	1	41	VAL	O-C-N	7.32	129.44	121.10
3	3	40	GLU	N-CA-C	7.31	121.10	110.28
1	1	164	SER	O-C-N	7.30	129.86	122.12
2	2	132	PRO	CA-C-O	-7.30	112.55	121.31
2	2	226	VAL	N-CA-C	7.29	118.38	108.17
1	1	121	THR	N-CA-C	7.29	119.30	111.36
2	2	192	GLN	O-C-N	7.25	131.68	123.27
2	2	229	VAL	O-C-N	7.24	130.85	122.81
1	1	103	ASN	O-C-N	7.22	129.78	122.12
2	2	19	ALA	O-C-N	7.21	131.55	123.40
2	2	120	GLN	O-C-N	7.19	131.74	122.39
1	1	210	THR	O-C-N	7.18	131.18	122.35
4	4	35	ASP	O-C-N	7.18	131.85	123.02
3	3	109	LEU	O-C-N	7.18	131.38	123.27
3	3	129	TYR	O-C-N	7.17	131.73	123.27
4	4	20	VAL	N-CA-C	7.17	118.20	107.80
3	3	154	GLY	O-C-N	7.17	130.69	123.88
3	3	184	VAL	CB-CA-C	-7.16	100.23	110.82
1	1	115	LEU	O-C-N	7.16	129.82	122.09
3	3	51	PRO	O-C-N	7.15	131.24	123.01
2	2	55	LYS	O-C-N	7.15	131.42	122.55
1	1	91	VAL	CA-C-O	-7.15	114.38	121.67
3	3	95	LEU	O-C-N	7.14	129.72	122.08
3	3	183	SER	O-C-N	7.13	129.45	122.03
2	2	122	HIS	O-C-N	7.13	131.30	123.10
3	3	111	PHE	N-CA-C	7.12	119.88	108.41
3	3	30	ILE	O-C-N	7.12	130.43	122.67
1	1	88	LYS	N-CA-C	7.10	120.53	109.52
2	2	209	VAL	O-C-N	7.10	130.60	123.00
3	3	29	THR	O-C-N	7.09	131.29	123.13
3	3	70	THR	N-CA-C	7.09	117.39	108.45
4	4	33	SER	O-C-N	7.09	131.62	122.97
3	3	137	PRO	CA-C-O	-7.08	113.26	121.34
1	1	40	ALA	N-CA-C	7.08	120.76	110.28
1	1	141	SER	N-CA-C	7.08	121.09	109.06
3	3	172	ARG	O-C-N	7.08	131.90	123.27
3	3	69	ALA	O-C-N	7.07	131.72	123.17
2	2	106	CYS	O-C-N	7.06	131.87	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	50	ASP	O-C-N	7.06	131.61	122.93
3	3	161	PHE	N-CA-C	7.06	120.23	108.73
2	2	160	PRO	O-C-N	7.05	131.44	122.91
2	2	91	GLU	O-C-N	7.05	130.22	122.11
3	3	56	ASN	N-CA-C	7.03	119.83	109.42
1	1	23	PRO	O-C-N	7.03	130.64	122.98
3	3	47	LEU	O-C-N	7.03	129.57	122.12
1	1	53	GLU	N-CA-C	7.03	121.56	112.92
2	2	96	PHE	O-C-N	7.02	129.31	122.07
2	2	75	GLU	N-CA-C	7.02	120.85	110.46
3	3	86	SER	O-C-N	7.02	129.56	122.12
3	3	5	VAL	N-CA-C	7.02	118.92	108.46
4	4	28	ASN	CB-CA-C	-7.01	99.10	110.74
3	3	205	ASN	O-C-N	7.00	132.11	123.01
3	3	223	PRO	O-C-N	7.00	130.61	122.98
1	1	25	LYS	N-CA-C	6.99	120.51	110.10
1	1	14	ASP	CA-C-O	-6.98	113.27	121.44
3	3	216	ASP	N-CA-C	6.98	118.54	111.07
1	1	220	ASP	O-C-N	6.98	131.13	123.10
2	2	104	TYR	O-C-N	6.98	129.26	122.07
3	3	5	VAL	O-C-N	6.97	130.56	123.10
2	2	68	ALA	O-C-N	6.97	130.36	123.46
2	2	69	SER	O-C-N	6.97	131.35	123.05
3	3	119	ALA	O-C-N	6.97	129.51	122.12
3	3	81	TYR	O-C-N	6.97	131.16	123.22
1	1	243	VAL	N-CA-C	6.97	119.58	108.85
3	3	59	SER	O-C-N	6.97	130.63	122.20
3	3	108	SER	N-CA-C	6.97	121.21	110.20
3	3	224	ILE	O-C-N	6.97	130.13	122.75
4	4	28	ASN	O-C-N	6.97	130.12	122.11
2	2	134	PHE	N-CA-C	6.96	119.91	109.25
2	2	252	VAL	CA-C-N	-6.96	116.41	123.10
2	2	252	VAL	C-N-CA	-6.96	116.41	123.10
2	2	214	THR	CA-C-O	-6.96	113.71	121.51
2	2	175	PHE	CA-CB-CG	-6.96	106.84	113.80
2	2	77	PHE	N-CA-C	6.96	125.61	110.80
2	2	24	THR	O-C-N	6.95	130.77	122.85
2	2	261	HIS	CA-C-O	-6.95	114.18	121.55
2	2	99	THR	O-C-N	6.94	130.07	122.15
1	1	61	ASN	O-C-N	6.94	131.69	123.36
1	1	131	VAL	N-CA-C	6.93	116.69	106.85
1	1	207	PHE	N-CA-C	6.92	120.61	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	119	SER	O-C-N	6.92	130.21	123.29
1	1	74	PRO	O-C-N	6.91	130.96	123.01
1	1	5	ALA	O-C-N	6.91	130.08	122.20
1	1	123	TYR	O-C-N	6.91	131.04	123.10
2	2	56	VAL	O-C-N	6.90	130.02	122.36
3	3	157	SER	O-C-N	6.90	130.29	122.22
1	1	157	GLN	CA-C-O	-6.89	113.35	120.80
2	2	100	LEU	O-C-N	6.89	129.16	122.07
2	2	117	ASN	N-CA-C	6.88	120.89	109.95
2	2	230	PHE	O-C-N	6.88	130.23	122.32
3	3	183	SER	N-CA-C	6.88	118.47	110.97
2	2	91	GLU	N-CA-C	6.88	122.72	111.37
2	2	111	ARG	O-C-N	6.88	132.19	123.12
2	2	17	ASP	O-C-N	6.87	131.30	123.27
3	3	1	SER	CA-C-N	-6.86	112.58	119.99
3	3	1	SER	C-N-CA	-6.86	112.58	119.99
2	2	156	THR	O-C-N	6.85	131.43	123.41
1	1	99	GLY	O-C-N	6.84	129.24	122.19
2	2	263	THR	O-C-N	6.83	132.10	123.01
3	3	114	VAL	N-CA-C	6.83	118.14	107.28
1	1	22	GLU	N-CA-C	6.83	124.90	109.81
3	3	23	VAL	O-C-N	6.83	128.58	121.07
3	3	125	PHE	N-CA-C	6.82	120.79	109.95
3	3	148	TYR	N-CA-C	6.82	119.43	109.07
3	3	162	THR	O-C-N	6.82	131.16	123.05
3	3	168	PRO	O-C-N	6.81	130.41	122.23
4	4	16	GLY	O-C-N	6.81	128.67	122.81
1	1	63	LEU	O-C-N	6.81	129.02	121.87
1	1	51	ASN	O-C-N	6.81	131.64	122.59
3	3	2	PRO	O-C-N	6.80	131.62	123.06
1	1	31	THR	O-C-N	6.79	130.71	122.35
3	3	72	SER	O-C-N	6.79	130.69	123.42
2	2	58	ALA	O-C-N	6.79	129.94	122.20
3	3	204	VAL	O-C-N	6.79	129.80	122.06
2	2	67	LEU	O-C-N	6.78	130.19	122.19
2	2	57	LEU	O-C-N	6.78	129.91	122.11
1	1	67	CYS	O-C-N	6.77	131.20	123.48
2	2	265	ILE	O-C-N	6.77	129.27	121.96
2	2	182	ASN	N-CA-C	6.76	120.68	108.17
1	1	75	SER	N-CA-C	6.76	119.44	109.24
1	1	183	ILE	O-C-N	6.76	130.27	123.18
1	1	17	VAL	O-C-N	6.75	129.16	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	76	ALA	O-C-N	6.75	130.67	123.11
1	1	98	SER	O-C-N	6.75	131.16	123.06
3	3	148	TYR	O-C-N	6.75	130.94	123.25
2	2	261	HIS	O-C-N	6.74	131.10	122.81
1	1	191	SER	O-C-N	6.74	130.81	121.64
3	3	217	ASP	O-C-N	6.74	130.10	122.22
2	2	74	GLN	O-C-N	6.73	131.30	122.95
2	2	23	ALA	N-CA-C	6.73	119.70	108.13
2	2	55	LYS	CB-CA-C	-6.73	102.34	111.89
2	2	43	GLU	CB-CA-C	-6.72	98.56	109.72
3	3	74	PRO	O-C-N	6.71	131.70	122.64
1	1	24	VAL	O-C-N	6.71	128.89	122.05
1	1	147	PRO	O-C-N	6.71	131.33	123.01
2	2	245	ILE	O-C-N	6.71	130.16	122.99
2	2	147	PRO	O-C-N	6.70	131.17	122.86
2	2	229	VAL	CB-CA-C	-6.70	102.44	111.15
4	4	38	ALA	O-C-N	6.70	131.50	122.59
1	1	17	VAL	CB-CA-C	-6.70	103.23	111.87
2	2	80	ILE	O-C-N	6.70	130.44	123.20
3	3	48	CYS	O-C-N	6.70	130.06	122.22
3	3	161	PHE	O-C-N	6.70	130.86	123.22
1	1	139	VAL	CB-CA-C	-6.69	101.84	111.34
1	1	128	GLU	O-C-N	6.69	130.96	122.93
2	2	45	PRO	O-C-N	6.69	130.12	123.03
1	1	101	THR	O-C-N	6.68	128.98	122.03
3	3	17	THR	O-C-N	6.68	130.47	122.26
4	4	24	ASN	O-C-N	6.68	129.76	121.95
1	1	102	THR	CA-C-O	-6.67	114.13	121.87
1	1	27	PRO	O-C-N	6.66	131.45	122.99
1	1	101	THR	N-CA-C	6.66	118.23	110.97
1	1	250	LEU	O-C-N	6.66	131.05	123.06
1	1	252	PHE	O-C-N	6.65	129.54	121.29
2	2	28	SER	O-C-N	6.65	130.46	122.21
1	1	132	SER	N-CA-C	6.65	120.08	109.24
1	1	72	PRO	O-C-N	6.65	130.79	122.22
2	2	52	ALA	O-C-N	6.64	130.98	122.81
2	2	226	VAL	O-C-N	6.64	130.16	123.18
3	3	135	GLY	O-C-N	6.63	129.73	122.70
1	1	97	ARG	N-CA-C	6.63	120.42	108.69
1	1	176	VAL	O-C-N	6.62	129.54	123.19
1	1	36	PHE	O-C-N	6.62	128.88	122.07
1	1	233	SER	O-C-N	6.62	130.78	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	137	GLY	O-C-N	6.61	129.48	122.93
1	1	35	PHE	N-CA-C	6.61	119.04	111.11
1	1	188	PRO	CA-C-O	-6.61	113.61	121.67
1	1	108	THR	O-C-N	6.59	130.45	123.06
1	1	198	ALA	O-C-N	6.59	129.94	122.22
2	2	53	THR	O-C-N	6.59	130.71	123.13
2	2	132	PRO	O-C-N	6.59	131.01	123.10
3	3	14	PHE	N-CA-C	6.59	119.98	109.24
1	1	8	GLY	O-C-N	6.58	130.27	122.50
1	1	153	ASP	O-C-N	6.58	131.34	122.59
2	2	96	PHE	N-CA-C	6.58	118.11	111.07
2	2	161	GLN	O-C-N	6.58	130.69	123.13
1	1	90	PRO	O-C-N	6.58	131.34	122.99
1	1	156	ASP	N-CA-C	6.58	119.77	110.50
3	3	110	ASN	O-C-N	6.58	130.88	123.05
3	3	221	ARG	N-CA-C	6.58	118.76	108.96
2	2	134	PHE	CB-CA-C	-6.57	99.51	110.29
2	2	190	PRO	O-C-N	6.57	131.51	122.64
2	2	127	LEU	O-C-N	6.57	130.95	122.87
2	2	61	ARG	O-C-N	6.57	130.60	122.92
3	3	99	ALA	N-CA-C	6.57	119.27	111.33
3	3	200	SER	CA-C-O	-6.56	114.65	121.87
4	4	33	SER	CA-C-O	-6.56	113.93	121.15
1	1	206	ASP	O-C-N	6.56	131.76	123.23
2	2	249	ILE	O-C-N	6.56	130.31	123.03
3	3	94	MET	O-C-N	6.56	129.07	122.12
3	3	58	ASN	CA-C-O	-6.55	113.99	121.72
3	3	106	ARG	O-C-N	6.55	131.07	123.41
1	1	232	ALA	O-C-N	6.54	131.25	123.33
2	2	177	ALA	O-C-N	6.54	130.62	123.10
3	3	58	ASN	O-C-N	6.54	130.27	122.94
1	1	147	PRO	CA-C-O	-6.54	113.98	121.56
2	2	140	THR	O-C-N	6.54	131.06	123.02
2	2	239	SER	O-C-N	6.54	130.91	122.87
2	2	203	ASP	O-C-N	6.53	130.84	123.27
1	1	126	ASP	CA-C-O	-6.53	113.70	121.66
3	3	110	ASN	CB-CA-C	-6.52	100.35	110.78
1	1	249	THR	O-C-N	6.52	130.28	122.85
1	1	107	MET	O-C-N	6.51	129.58	122.15
2	2	191	HIS	O-C-N	6.51	129.96	122.99
1	1	6	GLU	O-C-N	6.51	131.25	122.59
3	3	13	CYS	O-C-N	6.51	130.94	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	124	LYS	O-C-N	6.50	130.76	123.48
2	2	205	GLU	O-C-N	6.50	131.44	123.44
3	3	118	ALA	O-C-N	6.50	130.80	122.81
3	3	134	ALA	O-C-N	6.50	129.98	122.25
2	2	228	ALA	O-C-N	6.49	131.67	123.23
4	4	23	ASN	N-CA-C	6.49	124.63	110.80
1	1	182	GLN	O-C-N	6.49	131.19	123.27
1	1	140	ALA	O-C-N	6.49	131.88	123.06
2	2	193	ILE	O-C-N	6.47	130.21	123.03
3	3	212	VAL	O-C-N	6.47	129.92	123.00
3	3	121	VAL	O-C-N	6.46	130.33	122.83
1	1	60	GLU	O-C-N	6.46	130.53	123.10
1	1	168	THR	O-C-N	6.46	130.72	123.48
2	2	113	GLN	O-C-N	6.46	131.65	123.12
2	2	112	VAL	O-C-N	6.45	130.14	123.18
1	1	252	PHE	CB-CA-C	-6.44	102.74	110.15
2	2	105	LEU	N-CA-C	6.44	119.89	109.40
3	3	12	GLY	O-C-N	6.44	130.52	122.34
3	3	155	LEU	O-C-N	6.43	129.99	122.20
3	3	137	PRO	O-C-N	6.43	130.81	123.03
3	3	214	ALA	O-C-N	6.43	130.84	122.93
3	3	195	PRO	CA-C-N	-6.42	111.51	121.02
3	3	195	PRO	C-N-CA	-6.42	111.51	121.02
3	3	152	ASP	O-C-N	6.42	130.54	123.22
4	4	31	GLN	O-C-N	6.41	129.72	122.22
1	1	151	PRO	O-C-N	6.41	130.66	122.85
3	3	7	VAL	N-CA-C	6.41	117.65	107.98
2	2	22	SER	O-C-N	6.40	131.11	123.24
2	2	212	ALA	N-CA-C	6.40	119.64	108.82
3	3	61	ASN	CB-CA-C	-6.40	102.77	112.11
3	3	139	THR	O-C-N	6.40	130.89	123.41
1	1	59	GLN	N-CA-C	6.39	119.13	108.13
2	2	133	GLU	N-CA-C	6.38	120.33	111.90
3	3	4	ALA	O-C-N	6.38	130.78	122.93
2	2	252	VAL	O-C-N	6.38	129.63	122.68
1	1	142	VAL	O-C-N	6.38	130.15	123.26
3	3	171	TYR	O-C-N	6.37	131.43	123.15
2	2	27	GLN	O-C-N	6.37	129.98	122.34
2	2	227	VAL	O-C-N	6.37	131.22	122.88
1	1	152	ALA	O-C-N	6.36	130.66	122.39
1	1	193	LEU	O-C-N	6.36	130.15	122.96
2	2	63	TYR	O-C-N	6.36	130.57	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	98	VAL	CB-CA-C	-6.36	103.71	112.04
2	2	252	VAL	N-CA-C	6.36	117.58	107.98
1	1	78	PRO	O-C-N	6.35	131.22	122.64
2	2	54	ASP	O-C-N	6.35	130.35	122.92
2	2	116	CYS	O-C-N	6.35	131.04	122.59
1	1	227	GLN	CA-C-O	-6.35	113.91	120.89
1	1	95	TRP	O-C-N	6.34	130.21	123.42
1	1	19	PHE	O-C-N	6.34	131.40	123.15
1	1	29	ASN	CB-CA-C	-6.34	98.42	109.07
1	1	223	ARG	O-C-N	6.34	130.39	123.10
1	1	96	VAL	O-C-N	6.34	130.39	122.59
2	2	262	GLU	O-C-N	6.34	130.94	122.96
2	2	109	GLY	O-C-N	6.33	130.12	123.09
2	2	168	ARG	CA-C-O	-6.33	114.19	121.47
1	1	29	ASN	O-C-N	6.33	130.13	122.48
1	1	36	PHE	CB-CA-C	-6.32	100.95	110.88
3	3	8	ARG	N-CA-C	6.32	119.39	110.23
1	1	43	ILE	O-C-N	6.31	129.11	122.17
3	3	98	VAL	O-C-N	6.31	130.10	121.90
1	1	217	PRO	O-C-N	6.31	130.67	123.10
3	3	122	LYS	O-C-N	6.31	131.44	122.74
1	1	197	PRO	O-C-N	6.30	131.15	122.64
3	3	67	PHE	N-CA-C	6.30	119.29	109.52
2	2	66	ASP	O-C-N	6.30	130.41	123.04
2	2	253	ASN	CA-C-N	-6.30	113.19	119.93
2	2	253	ASN	C-N-CA	-6.30	113.19	119.93
2	2	32	ARG	O-C-N	6.29	131.06	123.13
2	2	150	PRO	O-C-N	6.29	131.14	122.64
3	3	116	THR	O-C-N	6.29	129.89	122.34
3	3	93	SER	O-C-N	6.29	130.07	122.96
1	1	251	PHE	O-C-N	6.29	130.64	122.97
2	2	31	GLY	O-C-N	6.29	130.66	122.87
1	1	48	PRO	O-C-N	6.28	129.83	122.98
2	2	82	ILE	N-CA-C	6.28	114.32	107.60
1	1	90	PRO	CA-C-O	-6.28	114.40	121.43
2	2	188	VAL	O-C-N	6.28	130.27	122.05
2	2	260	ARG	CA-C-N	-6.28	111.28	120.75
2	2	260	ARG	C-N-CA	-6.28	111.28	120.75
2	2	40	HIS	O-C-N	6.27	130.93	122.59
3	3	19	PRO	O-C-N	6.27	131.10	122.64
3	3	173	GLN	O-C-N	6.26	130.57	122.87
2	2	247	ALA	N-CA-C	6.26	119.45	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	136	LYS	O-C-N	6.26	128.44	121.43
1	1	130	THR	O-C-N	6.25	130.52	123.27
2	2	221	ALA	O-C-N	6.24	129.89	122.46
3	3	62	LYS	CA-C-O	-6.24	113.81	121.11
3	3	66	TYR	O-C-N	6.24	129.67	122.99
1	1	114	PHE	N-CA-C	6.24	119.74	111.75
1	1	88	LYS	O-C-N	6.23	131.25	123.15
1	1	201	PHE	N-CA-C	6.23	118.95	107.73
3	3	67	PHE	CA-C-O	-6.23	114.15	121.44
2	2	169	TYR	O-C-N	6.23	130.01	122.35
2	2	243	VAL	CB-CA-C	-6.23	102.89	110.99
1	1	226	ILE	O-C-N	6.23	129.63	122.97
2	2	208	TYR	O-C-N	6.23	130.29	123.13
2	2	180	HIS	O-C-N	6.23	130.59	122.93
3	3	70	THR	O-C-N	6.23	130.76	122.73
3	3	21	THR	O-C-N	6.23	129.97	122.68
2	2	185	GLN	O-C-N	6.22	129.66	122.25
2	2	108	THR	N-CA-C	6.22	118.53	109.07
2	2	195	ASN	N-CA-C	6.22	118.83	108.20
3	3	82	GLN	O-C-N	6.21	130.57	122.68
2	2	157	TRP	O-C-N	6.21	130.55	122.97
1	1	11	SER	O-C-N	6.21	130.59	122.89
2	2	65	ILE	O-C-N	6.21	129.83	123.00
1	1	195	VAL	O-C-N	6.21	130.04	123.02
2	2	88	LEU	O-C-N	6.21	129.64	122.25
1	1	166	GLY	O-C-N	6.21	129.69	122.68
2	2	224	THR	O-C-N	6.20	130.57	123.31
3	3	187	TRP	N-CA-C	6.20	119.64	109.72
1	1	64	ARG	O-C-N	6.20	130.29	123.22
1	1	46	LEU	O-C-N	6.19	130.59	123.29
1	1	236	ILE	O-C-N	6.19	129.20	122.76
1	1	245	CYS	O-C-N	6.18	128.43	121.32
1	1	102	THR	O-C-N	6.18	129.84	122.79
2	2	43	GLU	CA-C-O	-6.18	114.39	121.19
1	1	248	PRO	O-C-N	6.17	130.50	123.03
3	3	123	GLY	O-C-N	6.17	130.73	122.70
1	1	209	ASN	O-C-N	6.17	130.80	122.59
1	1	23	PRO	CA-C-O	-6.17	114.79	121.27
2	2	42	GLY	O-C-N	6.17	129.97	122.32
2	2	234	GLN	O-C-N	6.17	130.79	123.33
1	1	167	GLU	N-CA-C	6.16	119.19	109.39
3	3	46	GLU	CA-C-N	-6.15	111.95	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	46	GLU	C-N-CA	-6.15	111.95	120.38
3	3	162	THR	N-CA-C	6.15	118.72	108.20
1	1	229	ASN	O-C-N	6.15	130.32	122.39
3	3	138	THR	O-C-N	6.14	129.68	122.24
1	1	92	GLN	O-C-N	6.14	130.70	122.96
1	1	66	ASN	O-C-N	6.14	130.23	122.37
2	2	238	GLY	O-C-N	6.13	130.67	122.70
3	3	190	VAL	N-CA-C	6.13	116.69	107.80
1	1	175	LEU	O-C-N	6.13	130.38	123.27
1	1	247	ARG	N-CA-C	6.12	115.17	108.14
1	1	215	VAL	CB-CA-C	-6.11	102.70	111.19
3	3	7	VAL	O-C-N	6.11	129.33	122.68
1	1	39	ARG	O-C-N	6.10	130.71	123.33
2	2	62	TYR	O-C-N	6.10	130.15	123.13
1	1	177	GLY	O-C-N	6.10	130.63	122.70
2	2	201	THR	O-C-N	6.10	130.22	123.33
3	3	127	ILE	O-C-N	6.10	129.90	122.95
1	1	190	ASN	O-C-N	6.10	129.66	122.34
2	2	102	ARG	O-C-N	6.09	129.65	122.34
1	1	195	VAL	CA-C-O	-6.09	115.61	121.63
1	1	212	ASP	N-CA-C	6.09	120.03	112.24
3	3	200	SER	O-C-N	6.08	129.87	122.75
2	2	48	CYS	O-C-N	6.08	130.46	123.29
3	3	102	PHE	N-CA-C	6.08	119.39	109.24
3	3	160	VAL	O-C-N	6.08	131.69	122.76
1	1	156	ASP	O-C-N	6.07	130.03	122.86
2	2	247	ALA	O-C-N	6.07	130.51	123.41
2	2	230	PHE	CA-CB-CG	-6.07	107.73	113.80
3	3	165	PHE	N-CA-C	6.06	119.06	108.52
2	2	171	SER	O-C-N	6.05	130.51	122.04
3	3	69	ALA	CA-C-O	-6.05	114.56	121.40
3	3	224	ILE	N-CA-C	6.05	115.91	108.53
3	3	160	VAL	N-CA-C	6.05	116.52	107.51
1	1	157	GLN	O-C-N	6.04	131.35	123.07
1	1	170	ASN	CB-CA-C	-6.04	99.55	109.46
3	3	226	PRO	CA-C-N	-6.04	112.08	121.02
3	3	226	PRO	C-N-CA	-6.04	112.08	121.02
2	2	30	VAL	O-C-N	6.04	129.99	122.14
2	2	65	ILE	N-CA-C	6.04	117.62	108.80
2	2	95	VAL	CA-C-N	-6.04	112.59	120.44
2	2	95	VAL	C-N-CA	-6.04	112.59	120.44
1	1	129	VAL	O-C-N	6.03	129.72	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	31	SER	O-C-N	6.03	130.66	122.82
1	1	200	TRP	N-CA-C	6.03	119.31	109.24
3	3	76	THR	O-C-N	6.03	130.02	122.43
3	3	101	ASN	O-C-N	6.02	129.87	122.34
2	2	251	PRO	O-C-N	6.02	130.77	122.64
1	1	204	TRP	O-C-N	6.02	129.76	122.96
2	2	151	PHE	O-C-N	6.01	130.07	122.37
3	3	44	LEU	O-C-N	6.01	129.05	122.20
3	3	121	VAL	CB-CA-C	-6.01	102.97	111.21
2	2	129	PHE	O-C-N	6.01	130.53	122.96
3	3	10	HIS	O-C-N	6.01	130.06	122.37
3	3	113	PHE	O-C-N	6.01	130.38	123.29
1	1	81	THR	O-C-N	6.00	130.57	122.59
3	3	3	ILE	CB-CA-C	-6.00	104.06	111.08
1	1	206	ASP	CA-C-N	-6.00	111.62	120.38
1	1	206	ASP	C-N-CA	-6.00	111.62	120.38
2	2	205	GLU	N-CA-C	6.00	119.28	108.48
1	1	32	ARG	N-CA-C	6.00	119.42	109.46
1	1	227	GLN	O-C-N	6.00	130.19	123.48
2	2	248	SER	O-C-N	5.99	130.18	123.05
3	3	43	ASP	N-CA-C	5.99	118.18	108.41
1	1	61	ASN	CB-CA-C	-5.99	103.28	110.94
3	3	209	LEU	O-C-N	5.99	130.37	122.95
3	3	153	LEU	O-C-N	5.98	129.92	122.86
2	2	86	HIS	CA-CB-CG	-5.98	107.82	113.80
1	1	54	SER	O-C-N	5.97	131.29	122.81
2	2	151	PHE	CA-CB-CG	-5.96	107.84	113.80
3	3	43	ASP	O-C-N	5.96	130.19	123.27
2	2	101	ARG	O-C-N	5.96	130.13	122.39
2	2	207	PRO	O-C-N	5.95	130.67	122.64
3	3	57	PRO	N-CA-C	5.95	119.78	110.80
3	3	228	LYS	O-C-N	5.95	130.23	122.97
3	3	192	GLN	CA-C-O	-5.95	113.59	120.49
1	1	144	ARG	O-C-N	5.94	130.30	123.29
4	4	26	TYR	CA-C-O	-5.94	113.83	120.54
2	2	167	TYR	N-CA-C	5.94	118.59	108.02
3	3	159	PHE	CB-CA-C	-5.94	101.57	110.24
4	4	34	ILE	O-C-N	5.94	129.48	122.83
2	2	232	PRO	O-C-N	5.94	130.43	122.89
3	3	169	THR	O-C-N	5.94	129.93	123.10
1	1	110	GLN	O-C-N	5.94	130.49	122.59
3	3	206	SER	O-C-N	5.94	130.05	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	246	PRO	O-C-N	5.93	130.42	122.89
2	2	257	ASN	N-CA-C	5.93	118.71	109.52
2	2	49	ALA	O-C-N	5.93	130.27	122.33
3	3	8	ARG	O-C-N	5.93	130.16	122.87
1	1	137	ASP	CA-C-N	-5.92	111.72	121.97
1	1	137	ASP	C-N-CA	-5.92	111.72	121.97
2	2	89	ALA	O-C-N	5.92	130.37	122.43
1	1	235	ARG	NE-CZ-NH2	5.92	124.53	119.20
4	4	28	ASN	N-CA-C	5.92	121.14	111.37
1	1	136	THR	N-CA-C	5.92	121.23	113.30
2	2	112	VAL	CB-CA-C	-5.92	101.80	110.62
3	3	118	ALA	N-CA-C	5.92	118.39	110.35
1	1	34	ALA	N-CA-C	5.91	118.23	111.02
2	2	249	ILE	N-CA-C	5.91	116.81	108.36
3	3	58	ASN	CB-CA-C	-5.91	99.50	109.83
1	1	59	GLN	O-C-N	5.90	131.43	123.34
2	2	260	ARG	N-CA-C	5.90	116.34	108.38
3	3	145	GLN	O-C-N	5.90	130.60	122.46
2	2	25	ASN	N-CA-C	5.89	117.98	108.32
2	2	246	THR	O-C-N	5.89	131.16	122.97
1	1	76	PHE	CA-C-O	-5.89	114.52	121.06
3	3	42	SER	O-C-N	5.89	130.38	122.49
2	2	124	GLY	O-C-N	5.88	130.35	122.70
2	2	186	TRP	O-C-N	5.88	128.90	122.20
2	2	108	THR	O-C-N	5.88	129.95	123.25
3	3	68	SER	O-C-N	5.88	130.57	123.16
3	3	18	ASN	N-CA-C	5.88	118.06	109.71
3	3	229	TRP	N-CA-C	5.88	117.89	109.14
3	3	49	LYS	O-C-N	5.88	130.75	122.41
3	3	117	GLY	CA-C-O	-5.88	115.29	122.75
1	1	62	ASP	O-C-N	5.87	129.83	122.55
2	2	139	GLY	O-C-N	5.87	130.26	123.51
2	2	29	THR	O-C-N	5.87	130.03	122.81
3	3	34	ASN	O-C-N	5.87	130.06	122.19
2	2	204	LEU	O-C-N	5.86	130.81	123.19
1	1	201	PHE	O-C-N	5.86	128.85	122.64
2	2	59	ALA	O-C-N	5.86	130.73	122.41
3	3	6	THR	O-C-N	5.86	129.96	122.93
1	1	244	PHE	O-C-N	5.86	130.26	123.17
3	3	10	HIS	N-CA-C	5.86	119.49	112.93
2	2	20	GLY	O-C-N	5.86	130.63	122.55
3	3	193	LEU	O-C-N	5.85	129.25	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	111	PHE	O-C-N	5.85	129.95	122.93
2	2	136	THR	O-C-N	5.85	129.21	122.25
4	4	18	GLU	O-C-N	5.85	130.05	123.27
1	1	61	ASN	N-CA-C	5.84	117.66	107.49
2	2	51	THR	O-C-N	5.84	130.78	123.01
3	3	202	THR	CB-CA-C	-5.83	101.54	109.42
3	3	208	ILE	O-C-N	5.83	130.52	122.88
1	1	150	ALA	N-CA-C	5.82	118.12	110.08
2	2	147	PRO	CA-C-O	-5.82	114.10	122.31
4	4	37	SER	N-CA-C	5.82	117.78	108.41
1	1	4	ASN	O-C-N	5.82	130.03	123.28
2	2	164	PRO	O-C-N	5.81	130.49	122.64
3	3	28	LYS	CB-CA-C	-5.81	101.88	111.36
2	2	107	LYS	O-C-N	5.81	130.07	123.27
1	1	165	LEU	O-C-N	5.81	128.28	122.12
4	4	32	ASN	CA-C-N	-5.81	112.71	120.90
4	4	32	ASN	C-N-CA	-5.81	112.71	120.90
3	3	112	LEU	O-C-N	5.81	129.81	123.13
2	2	241	SER	O-C-N	5.80	130.47	122.46
1	1	80	SER	O-C-N	5.80	130.19	123.41
2	2	176	PHE	O-C-N	5.80	129.62	123.42
2	2	244	GLN	CB-CA-C	-5.79	99.69	109.83
1	1	142	VAL	N-CA-C	5.79	116.22	108.11
2	2	95	VAL	N-CA-C	5.79	116.53	110.62
2	2	189	TYR	CA-C-N	-5.79	112.60	119.84
2	2	189	TYR	C-N-CA	-5.79	112.60	119.84
3	3	109	LEU	CA-C-O	-5.79	114.12	120.43
3	3	52	THR	CA-C-O	-5.79	114.87	121.58
2	2	191	HIS	CA-CB-CG	-5.79	108.02	113.80
2	2	38	GLU	O-C-N	5.78	129.19	123.46
4	4	30	TYR	O-C-N	5.78	130.78	122.28
1	1	84	PRO	O-C-N	5.78	130.44	122.64
2	2	113	GLN	CA-C-N	-5.78	115.14	122.37
2	2	113	GLN	C-N-CA	-5.78	115.14	122.37
1	1	184	SER	O-C-N	5.78	130.32	123.27
4	4	27	SER	O-C-N	5.78	130.02	122.97
3	3	125	PHE	O-C-N	5.78	130.44	123.16
3	3	121	VAL	N-CA-C	5.77	117.64	108.87
1	1	138	THR	O-C-N	5.77	130.04	122.89
2	2	229	VAL	N-CA-C	5.77	116.51	108.89
1	1	86	LYS	O-C-N	5.77	130.10	122.43
2	2	60	GLU	O-C-N	5.76	130.38	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	210	ASN	O-C-N	5.76	130.26	122.59
1	1	159	ILE	CB-CA-C	-5.76	103.24	111.31
2	2	128	VAL	O-C-N	5.76	131.23	122.76
1	1	2	SER	N-CA-C	5.76	118.58	110.23
3	3	220	LEU	O-C-N	5.76	130.32	123.24
3	3	24	PRO	O-C-N	5.76	130.41	122.64
3	3	207	ASP	O-C-N	5.76	129.78	123.27
1	1	49	GLY	O-C-N	5.75	129.96	122.71
1	1	207	PHE	CA-CB-CG	-5.75	108.05	113.80
1	1	192	PRO	O-C-N	5.75	129.94	122.24
2	2	82	ILE	CB-CA-C	-5.74	104.58	111.18
3	3	68	SER	N-CA-C	5.74	119.08	109.95
1	1	199	ALA	O-C-N	5.74	130.22	122.59
2	2	173	THR	CA-C-O	-5.74	114.93	121.58
1	1	121	THR	O-C-N	5.74	128.69	122.15
2	2	16	SER	O-C-N	5.74	130.27	123.27
2	2	153	MET	O-C-N	5.74	129.89	122.89
3	3	219	THR	N-CA-C	5.74	117.90	109.24
4	4	36	LEU	O-C-N	5.74	130.36	123.36
2	2	192	GLN	CA-C-O	-5.73	114.41	121.06
2	2	242	ASP	O-C-N	5.73	129.80	122.93
3	3	112	LEU	N-CA-C	5.73	118.07	108.96
3	3	196	LEU	O-C-N	5.73	130.63	123.01
1	1	45	MET	O-C-N	5.72	129.78	123.25
1	1	215	VAL	O-C-N	5.72	130.38	122.88
2	2	173	THR	O-C-N	5.72	130.78	122.94
3	3	57	PRO	O-C-N	5.72	129.51	123.10
1	1	56	PHE	O-C-N	5.72	129.91	122.87
1	1	230	THR	O-C-N	5.72	130.00	123.31
3	3	42	SER	N-CA-C	5.72	120.53	113.50
1	1	225	TRP	O-C-N	5.72	130.66	123.23
3	3	150	ILE	O-C-N	5.72	129.47	122.95
3	3	192	GLN	CB-CA-C	-5.72	100.91	110.29
3	3	189	THR	O-C-N	5.71	130.03	123.29
1	1	235	ARG	N-CA-C	5.71	119.03	109.95
1	1	24	VAL	N-CA-C	5.71	116.99	111.91
2	2	90	GLY	O-C-N	5.71	130.50	122.80
3	3	205	ASN	N-CA-C	5.71	118.86	107.62
1	1	21	ALA	N-CA-C	5.70	115.94	108.07
1	1	76	PHE	CB-CA-C	-5.70	100.22	110.03
2	2	144	ASP	N-CA-C	5.70	119.96	112.89
3	3	114	VAL	CB-CA-C	-5.70	103.58	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	20	ASP	O-C-N	5.70	130.07	123.17
3	3	106	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	2	225	LEU	O-C-N	5.69	129.76	122.93
3	3	40	GLU	O-C-N	5.69	129.83	122.89
3	3	107	GLY	O-C-N	5.69	130.36	123.37
1	1	133	ALA	N-CA-C	5.68	118.57	110.10
3	3	149	ALA	CA-C-N	-5.68	115.04	122.37
3	3	149	ALA	C-N-CA	-5.68	115.04	122.37
1	1	75	SER	O-C-N	5.68	130.04	123.17
2	2	71	THR	O-C-N	5.67	130.71	123.11
1	1	133	ALA	O-C-N	5.67	129.98	122.95
1	1	171	PRO	O-C-N	5.67	130.30	122.64
2	2	260	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	1	5	ALA	N-CA-C	5.67	119.00	111.75
1	1	223	ARG	NE-CZ-NH2	5.66	124.30	119.20
2	2	121	PHE	N-CA-C	5.66	120.31	113.17
3	3	188	VAL	O-C-N	5.66	131.08	122.76
2	2	166	GLY	O-C-N	5.66	128.28	122.90
1	1	178	ALA	O-C-N	5.66	129.85	123.06
1	1	53	GLU	CB-CA-C	-5.65	101.00	110.56
3	3	104	GLN	N-CA-C	5.65	117.99	109.23
1	1	228	GLY	CA-C-O	-5.64	116.85	121.76
1	1	139	VAL	O-C-N	5.64	129.38	122.72
2	2	257	ASN	O-C-N	5.64	130.48	123.15
1	1	163	PRO	CA-C-O	-5.63	114.33	120.92
1	1	243	VAL	O-C-N	5.63	128.95	123.03
1	1	94	ARG	O-C-N	5.63	129.38	122.34
3	3	111	PHE	CB-CA-C	-5.63	101.52	110.81
3	3	9	GLU	O-C-N	5.63	130.08	122.59
1	1	3	ASP	N-CA-C	5.63	116.00	108.23
1	1	109	LYS	O-C-N	5.63	129.57	123.10
1	1	213	PHE	CB-CA-C	-5.63	101.40	109.84
2	2	79	HIS	O-C-N	5.63	129.57	123.10
2	2	65	ILE	CB-CA-C	-5.63	102.49	110.82
3	3	52	THR	O-C-N	5.62	130.64	122.94
3	3	124	LYS	O-C-N	5.61	130.12	123.27
3	3	166	ILE	O-C-N	5.61	131.01	122.76
1	1	169	ARG	O-C-N	5.61	130.62	122.43
2	2	223	TRP	O-C-N	5.61	130.53	123.23
3	3	84	ALA	O-C-N	5.61	130.05	122.59
1	1	186	VAL	O-C-N	5.60	129.31	123.26
1	1	252	PHE	N-CA-C	5.60	118.51	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	239	LYS	O-C-N	5.60	129.60	123.22
2	2	131	ALA	N-CA-C	5.60	119.28	109.48
2	2	21	ASN	O-C-N	5.60	129.54	122.37
2	2	33	LEU	O-C-N	5.60	130.32	122.77
1	1	194	SER	O-C-N	5.59	128.52	122.15
2	2	125	SER	O-C-N	5.59	129.85	123.48
3	3	39	GLY	O-C-N	5.59	129.78	122.35
1	1	97	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	1	237	ARG	NE-CZ-NH2	5.57	124.22	119.20
2	2	168	ARG	O-C-N	5.57	129.26	122.96
3	3	77	SER	O-C-N	5.57	129.44	122.86
2	2	15	ALA	O-C-N	5.57	129.73	123.27
1	1	19	PHE	CB-CA-C	-5.57	98.38	109.79
2	2	197	ARG	O-C-N	5.56	130.13	122.46
1	1	122	TYR	O-C-N	5.55	130.07	123.24
1	1	202	ASN	N-CA-C	5.55	122.63	110.80
2	2	23	ALA	O-C-N	5.55	130.95	123.34
1	1	132	SER	O-C-N	5.55	129.54	123.27
3	3	28	LYS	O-C-N	5.55	132.25	122.09
1	1	57	VAL	N-CA-C	5.55	116.27	108.17
2	2	13	ARG	O-C-N	5.55	130.03	122.37
2	2	110	TRP	O-C-N	5.55	130.04	123.27
2	2	115	GLN	O-C-N	5.55	130.26	123.21
3	3	108	SER	O-C-N	5.55	129.56	123.01
3	3	67	PHE	O-C-N	5.55	130.36	123.15
3	3	91	CYS	O-C-N	5.55	129.97	122.59
1	1	185	PHE	CA-C-O	-5.54	115.35	121.28
1	1	189	TYR	O-C-N	5.54	129.96	122.59
3	3	135	GLY	CA-C-O	-5.54	117.24	122.39
1	1	251	PHE	CB-CA-C	-5.54	100.79	109.70
2	2	73	THR	N-CA-C	5.53	117.31	111.28
2	2	50	ASP	CA-C-N	-5.53	112.83	121.02
2	2	50	ASP	C-N-CA	-5.53	112.83	121.02
1	1	93	TRP	O-C-N	5.53	129.13	122.94
2	2	200	THR	O-C-N	5.53	130.00	122.37
2	2	144	ASP	O-C-N	5.52	130.08	122.46
1	1	143	LEU	O-C-N	5.52	129.68	123.27
3	3	125	PHE	CB-CA-C	-5.52	99.26	109.37
1	1	161	TYR	O-C-N	5.52	129.77	122.04
3	3	164	PRO	CA-C-O	-5.52	115.05	121.34
1	1	247	ARG	CA-C-O	-5.52	115.91	120.71
1	1	253	PRO	O-C-N	5.52	130.09	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	201	THR	N-CA-C	5.52	117.66	108.99
2	2	243	VAL	O-C-N	5.52	128.89	122.99
1	1	234	VAL	CA-C-N	-5.51	113.99	122.87
1	1	234	VAL	C-N-CA	-5.51	113.99	122.87
1	1	135	GLY	O-C-N	5.51	129.21	123.09
3	3	25	ILE	N-CA-C	5.51	120.00	113.22
3	3	142	GLN	CA-C-N	-5.51	113.10	120.54
3	3	142	GLN	C-N-CA	-5.51	113.10	120.54
1	1	221	PHE	O-C-N	5.50	129.41	122.37
2	2	172	ARG	CA-C-O	-5.50	114.90	121.89
1	1	64	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	2	52	ALA	CA-C-N	-5.49	114.89	122.30
2	2	52	ALA	C-N-CA	-5.49	114.89	122.30
2	2	227	VAL	CB-CA-C	-5.49	103.56	111.19
2	2	222	ASN	O-C-N	5.49	128.65	122.22
2	2	119	SER	N-CA-C	5.49	116.49	108.14
2	2	130	MET	O-C-N	5.49	129.83	123.30
1	1	20	VAL	O-C-N	5.49	129.43	122.57
1	1	167	GLU	O-C-N	5.49	129.75	122.56
2	2	220	HIS	O-C-N	5.49	130.86	123.34
1	1	9	LYS	CA-C-N	-5.49	114.90	122.69
1	1	9	LYS	C-N-CA	-5.49	114.90	122.69
2	2	114	VAL	O-C-N	5.49	129.63	122.94
1	1	234	VAL	O-C-N	5.48	130.06	122.88
1	1	238	TYR	N-CA-C	5.48	117.40	108.63
1	1	39	ARG	NE-CZ-NH2	5.46	124.12	119.20
4	4	37	SER	O-C-N	5.46	129.49	122.93
1	1	181	THR	O-C-N	5.46	128.61	122.27
2	2	219	GLN	N-CA-C	5.46	119.73	112.30
2	2	155	THR	O-C-N	5.46	129.17	122.34
3	3	15	TYR	O-C-N	5.46	130.01	123.13
3	3	71	ASN	O-C-N	5.46	129.85	122.59
1	1	180	ASN	O-C-N	5.46	129.53	122.43
3	3	28	LYS	CA-C-N	-5.46	114.93	122.30
3	3	28	LYS	C-N-CA	-5.46	114.93	122.30
4	4	18	GLU	N-CA-C	5.46	117.31	108.41
2	2	189	TYR	CA-C-O	-5.45	115.02	120.64
1	1	44	GLY	O-C-N	5.45	129.74	123.58
2	2	115	GLN	N-CA-C	5.45	118.37	109.59
3	3	60	ASN	O-C-N	5.45	129.83	122.59
3	3	23	VAL	CB-CA-C	-5.44	105.01	110.89
1	1	144	ARG	NE-CZ-NH2	5.44	124.09	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	123	ALA	O-C-N	5.44	130.26	123.19
1	1	116	CYS	O-C-N	5.43	129.71	122.43
3	3	215	GLY	O-C-N	5.43	128.19	122.59
1	1	127	LEU	N-CA-C	5.43	117.26	108.41
1	1	40	ALA	O-C-N	5.43	129.51	122.89
2	2	232	PRO	N-CA-C	5.43	119.73	111.15
3	3	89	CYS	O-C-N	5.43	129.44	122.39
1	1	235	ARG	O-C-N	5.42	130.00	123.16
1	1	179	GLY	O-C-N	5.42	129.13	122.46
3	3	53	PHE	CB-CA-C	-5.42	101.22	109.89
2	2	264	VAL	O-C-N	5.42	129.34	122.57
3	3	147	THR	O-C-N	5.41	129.78	122.96
1	1	127	LEU	O-C-N	5.41	129.55	123.27
2	2	94	GLY	O-C-N	5.41	129.73	122.70
2	2	29	THR	N-CA-C	5.41	117.70	110.35
3	3	125	PHE	CA-C-O	-5.40	115.05	121.16
3	3	159	PHE	O-C-N	5.40	130.74	123.34
1	1	224	LEU	N-CA-C	5.40	117.77	109.07
2	2	54	ASP	N-CA-C	5.40	116.19	108.74
3	3	221	ARG	NE-CZ-NH2	5.40	124.06	119.20
3	3	165	PHE	CB-CA-C	-5.40	103.19	111.83
2	2	250	GLN	N-CA-C	5.40	118.97	107.91
1	1	61	ASN	CA-C-N	-5.39	114.70	122.36
1	1	61	ASN	C-N-CA	-5.39	114.70	122.36
2	2	126	LEU	O-C-N	5.39	130.24	123.23
3	3	224	ILE	CB-CA-C	-5.39	103.04	110.91
2	2	125	SER	N-CA-C	5.39	117.28	108.55
1	1	219	ALA	O-C-N	5.38	129.75	122.59
1	1	42	PRO	O-C-N	5.38	129.20	123.01
2	2	237	SER	O-C-N	5.38	129.52	123.06
1	1	113	ALA	CA-C-N	-5.38	112.53	120.38
1	1	113	ALA	C-N-CA	-5.38	112.53	120.38
2	2	96	PHE	CB-CA-C	-5.38	102.43	110.88
3	3	107	GLY	N-CA-C	5.38	118.59	111.70
1	1	247	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	3	172	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	1	145	TRP	O-C-N	5.37	130.18	123.19
2	2	39	ALA	O-C-N	5.37	130.17	123.19
2	2	77	PHE	O-C-N	5.37	129.73	122.59
2	2	25	ASN	O-C-N	5.37	129.54	123.42
3	3	8	ARG	NE-CZ-NH2	5.36	124.03	119.20
2	2	13	ARG	NE-CZ-NH2	5.36	124.03	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	24	THR	CA-C-O	-5.36	115.48	121.81
3	3	210	THR	N-CA-C	5.36	117.40	108.02
3	3	227	THR	O-C-N	5.35	130.12	123.01
2	2	111	ARG	NE-CZ-NH2	5.34	124.01	119.20
3	3	189	THR	N-CA-C	5.34	117.67	109.07
1	1	117	PHE	CB-CA-C	-5.34	102.94	111.86
2	2	61	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	1	136	THR	O-C-N	5.34	128.70	122.24
2	2	81	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	2	32	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	2	75	GLU	CA-C-N	-5.34	113.23	121.56
2	2	75	GLU	C-N-CA	-5.34	113.23	121.56
3	3	140	ARG	NE-CZ-NH2	5.34	124.00	119.20
3	3	184	VAL	O-C-N	5.34	128.87	123.00
1	1	222	GLY	CA-C-N	-5.34	113.12	121.87
1	1	222	GLY	C-N-CA	-5.34	113.12	121.87
1	1	170	ASN	CA-C-N	-5.33	113.17	119.84
1	1	170	ASN	C-N-CA	-5.33	113.17	119.84
2	2	41	HIS	O-C-N	5.33	129.73	122.37
1	1	169	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	3	124	LYS	N-CA-C	5.33	118.14	109.24
2	2	55	LYS	CA-C-N	-5.33	116.09	122.22
2	2	55	LYS	C-N-CA	-5.33	116.09	122.22
3	3	103	ASN	O-C-N	5.32	128.82	122.27
3	3	65	PRO	O-C-N	5.32	129.82	122.64
3	3	115	PHE	CB-CA-C	-5.32	102.58	110.67
2	2	26	THR	O-C-N	5.32	129.77	123.33
2	2	121	PHE	O-C-N	5.32	128.99	122.34
3	3	221	ARG	O-C-N	5.32	129.22	123.10
1	1	214	GLY	O-C-N	5.32	128.93	122.60
3	3	185	ASP	O-C-N	5.31	129.14	121.97
1	1	16	SER	O-C-N	5.31	129.24	122.33
1	1	141	SER	O-C-N	5.31	129.76	123.33
4	4	24	ASN	CB-CA-C	-5.31	102.45	111.26
2	2	46	ALA	O-C-N	5.31	129.65	122.59
1	1	111	ASP	O-C-N	5.31	128.77	122.46
3	3	159	PHE	CA-C-N	-5.30	115.98	122.93
3	3	159	PHE	C-N-CA	-5.30	115.98	122.93
1	1	26	LEU	CA-C-N	-5.30	114.48	119.89
1	1	26	LEU	C-N-CA	-5.30	114.48	119.89
3	3	110	ASN	N-CA-C	5.30	117.27	108.20
1	1	18	ASP	O-C-N	5.30	129.72	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	201	GLY	O-C-N	5.30	129.03	122.41
2	2	21	ASN	N-CA-C	5.29	118.86	112.93
1	1	234	VAL	CB-CA-C	-5.29	103.83	111.19
4	4	29	GLN	O-C-N	5.29	129.52	122.43
3	3	100	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	2	236	ALA	CA-C-O	-5.28	115.95	121.55
3	3	33	PRO	O-C-N	5.28	129.29	122.85
2	2	218	THR	O-C-N	5.28	129.61	122.59
2	2	226	VAL	CB-CA-C	-5.28	102.97	110.83
3	3	205	ASN	CB-CA-C	-5.27	102.15	111.22
1	1	204	TRP	CA-C-O	-5.27	115.41	121.47
1	1	33	VAL	O-C-N	5.26	129.15	122.57
1	1	52	ILE	O-C-N	5.26	129.26	122.26
1	1	96	VAL	CA-C-O	-5.26	115.12	121.54
1	1	69	LEU	N-CA-C	5.26	117.30	109.25
3	3	93	SER	CA-C-O	-5.26	115.42	121.47
3	3	218	PHE	CB-CA-C	-5.25	101.96	109.84
2	2	256	PHE	CB-CA-C	-5.25	101.08	109.75
3	3	38	CYS	CA-C-O	-5.25	114.64	121.73
3	3	164	PRO	CA-C-N	-5.25	113.86	122.26
3	3	164	PRO	C-N-CA	-5.25	113.86	122.26
1	1	119	PRO	O-C-N	5.25	129.72	122.64
2	2	64	THR	O-C-N	5.25	129.16	123.13
3	3	110	ASN	CA-C-O	-5.24	115.09	120.54
2	2	95	VAL	CB-CA-C	-5.23	105.07	112.14
2	2	103	HIS	O-C-N	5.23	129.66	123.27
2	2	186	TRP	N-CA-C	5.23	118.45	111.75
3	3	27	GLY	O-C-N	5.23	128.51	122.60
3	3	36	TYR	O-C-N	5.23	129.44	122.43
3	3	190	VAL	O-C-N	5.23	129.22	123.10
2	2	101	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	2	197	ARG	NE-CZ-NH2	5.23	123.91	119.20
3	3	104	GLN	O-C-N	5.23	129.33	123.27
3	3	170	HIS	O-C-N	5.23	128.33	122.22
1	1	106	LEU	O-C-N	5.22	129.30	123.19
4	4	19	GLY	O-C-N	5.22	129.49	122.70
3	3	50	LEU	CA-C-N	-5.22	114.19	119.83
3	3	50	LEU	C-N-CA	-5.22	114.19	119.83
2	2	194	LEU	O-C-N	5.22	129.22	122.43
3	3	156	ASN	O-C-N	5.22	129.54	122.96
3	3	160	VAL	CA-C-N	-5.22	115.83	122.77
3	3	160	VAL	C-N-CA	-5.22	115.83	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	161	PHE	CA-C-N	-5.22	116.06	122.84
3	3	161	PHE	C-N-CA	-5.22	116.06	122.84
1	1	47	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	2	77	PHE	CA-CB-CG	-5.21	108.59	113.80
2	2	230	PHE	N-CA-C	5.21	119.53	111.56
1	1	225	TRP	CA-C-O	-5.21	115.07	120.70
2	2	26	THR	N-CA-C	5.21	117.91	109.06
3	3	188	VAL	CA-C-N	-5.21	115.82	123.00
3	3	188	VAL	C-N-CA	-5.21	115.82	123.00
2	2	79	HIS	CA-CB-CG	-5.20	108.60	113.80
2	2	18	LYS	O-C-N	5.20	129.08	123.10
2	2	72	THR	O-C-N	5.20	129.15	122.39
3	3	35	ASP	O-C-N	5.20	129.15	122.39
4	4	22	ILE	O-C-N	5.20	129.06	122.57
1	1	103	ASN	CB-CA-C	-5.19	101.85	110.68
3	3	100	ARG	O-C-N	5.19	129.63	122.46
1	1	69	LEU	O-C-N	5.19	129.41	123.02
3	3	80	ASP	N-CA-C	5.19	116.63	107.61
1	1	209	ASN	CB-CA-C	-5.18	100.10	110.42
2	2	183	GLN	O-C-N	5.18	129.49	122.59
2	2	216	SER	O-C-N	5.18	129.45	122.61
1	1	205	SER	O-C-N	5.18	129.77	122.41
2	2	220	HIS	N-CA-C	5.18	117.04	108.13
1	1	105	PRO	O-C-N	5.18	130.94	121.10
2	2	117	ASN	O-C-N	5.18	129.69	123.16
3	3	92	ASN	O-C-N	5.18	128.41	122.25
2	2	14	VAL	CB-CA-C	-5.18	104.06	111.31
2	2	230	PHE	CB-CA-C	-5.18	101.35	111.03
4	4	24	ASN	N-CA-C	5.17	119.05	112.12
2	2	175	PHE	O-C-N	5.17	129.46	122.59
3	3	78	LEU	O-C-N	5.17	128.04	122.15
2	2	233	LEU	O-C-N	5.17	129.35	122.95
1	1	67	CYS	CA-C-N	-5.16	113.77	122.29
1	1	67	CYS	C-N-CA	-5.16	113.77	122.29
3	3	60	ASN	CA-C-N	-5.16	115.20	122.63
3	3	60	ASN	C-N-CA	-5.16	115.20	122.63
3	3	115	PHE	O-C-N	5.16	129.74	122.77
3	3	211	LEU	O-C-N	5.16	129.66	123.16
1	1	65	LEU	N-CA-C	5.16	118.15	109.95
2	2	170	ASP	CA-C-N	-5.16	115.35	123.91
2	2	170	ASP	C-N-CA	-5.16	115.35	123.91
3	3	131	PRO	N-CA-C	5.16	115.42	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	240	SER	O-C-N	5.15	129.44	122.59
2	2	81	ARG	O-C-N	5.15	129.09	123.27
2	2	158	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	1	210	THR	CB-CA-C	-5.15	100.90	109.55
3	3	63	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	1	248	PRO	N-CA-C	5.14	119.16	111.14
2	2	102	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	1	56	PHE	CB-CA-C	-5.14	101.19	109.72
3	3	7	VAL	CB-CA-C	-5.14	105.68	111.23
2	2	152	THR	O-C-N	5.14	129.74	123.21
2	2	258	GLY	O-C-N	5.13	129.37	122.70
3	3	13	CYS	N-CA-C	5.13	117.66	109.96
1	1	172	HIS	O-C-N	5.13	129.85	123.19
1	1	233	SER	CA-C-N	-5.13	116.14	123.11
1	1	233	SER	C-N-CA	-5.13	116.14	123.11
3	3	188	VAL	CB-CA-C	-5.13	104.13	111.31
3	3	191	TRP	O-C-N	5.13	129.85	123.19
2	2	214	THR	O-C-N	5.12	129.41	122.96
2	2	195	ASN	O-C-N	5.12	129.14	123.05
2	2	235	TYR	N-CA-C	5.12	116.84	108.55
2	2	35	GLY	O-C-N	5.12	129.35	122.70
3	3	54	LEU	O-C-N	5.12	129.03	123.04
1	1	48	PRO	CA-C-O	-5.12	115.90	121.27
1	1	96	VAL	CB-CA-C	-5.12	104.57	111.63
1	1	208	GLY	O-C-N	5.11	129.88	122.26
1	1	185	PHE	CB-CA-C	-5.11	101.75	110.95
1	1	182	GLN	N-CA-C	5.11	117.77	109.24
2	2	128	VAL	CB-CA-C	-5.10	104.17	111.31
2	2	256	PHE	O-C-N	5.10	129.03	123.27
3	3	151	TRP	O-C-N	5.10	129.12	123.05
1	1	129	VAL	CB-CA-C	-5.09	103.91	110.84
2	2	127	LEU	CA-C-N	-5.09	116.26	122.93
2	2	127	LEU	C-N-CA	-5.09	116.26	122.93
3	3	55	GLY	O-C-N	5.09	129.32	122.70
3	3	53	PHE	O-C-N	5.09	129.19	122.93
2	2	219	GLN	O-C-N	5.09	129.23	122.26
3	3	146	ALA	CA-C-O	-5.09	114.08	120.84
4	4	25	PHE	CB-CA-C	-5.08	100.30	110.42
2	2	239	SER	CA-C-O	-5.08	115.60	121.19
3	3	139	THR	CA-C-N	-5.08	113.19	120.82
3	3	139	THR	C-N-CA	-5.08	113.19	120.82
3	3	158	SER	O-C-N	5.08	130.21	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	170	ASN	N-CA-C	5.08	116.90	109.84
3	3	113	PHE	CB-CA-C	-5.08	100.94	109.72
3	3	133	GLY	O-C-N	5.08	129.30	122.70
3	3	165	PHE	O-C-N	5.07	129.08	122.38
3	3	177	THR	O-C-N	5.07	129.12	122.33
2	2	47	SER	O-C-N	5.06	129.59	122.41
1	1	21	ALA	O-C-N	5.06	130.50	122.11
2	2	168	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	2	172	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	1	70	LEU	N-CA-C	5.05	117.31	108.52
2	2	118	ALA	O-C-N	5.05	129.31	122.59
3	3	38	CYS	O-C-N	5.05	130.04	122.76
3	3	120	MET	O-C-N	5.05	129.43	122.46
1	1	149	GLY	O-C-N	5.05	129.04	122.42
3	3	77	SER	N-CA-C	5.05	117.62	110.50
3	3	204	VAL	N-CA-C	5.05	119.16	111.89
3	3	214	ALA	CA-C-O	-5.05	115.00	120.81
3	3	1	SER	O-C-N	5.05	131.08	123.00
3	3	176	TYR	O-C-N	5.05	129.30	122.59
2	2	64	THR	N-CA-C	5.04	116.98	108.96
2	2	152	THR	CA-C-O	-5.04	115.36	120.71
1	1	21	ALA	CB-CA-C	-5.04	102.81	114.41
1	1	94	ARG	NE-CZ-NH2	5.04	123.73	119.20
3	3	11	LYS	O-C-N	5.04	129.00	122.81
2	2	133	GLU	CB-CA-C	-5.03	103.76	111.66
2	2	34	CYS	O-C-N	5.03	129.06	122.87
2	2	165	THR	O-C-N	5.03	128.88	122.39
2	2	154	ASP	O-C-N	5.02	129.95	123.07
1	1	201	PHE	CB-CA-C	-5.02	103.95	111.73
3	3	90	MET	O-C-N	5.02	129.53	122.41
1	1	89	ALA	N-CA-C	5.01	116.01	109.64
4	4	20	VAL	O-C-N	5.01	128.97	123.10
1	1	37	TYR	O-C-N	5.01	129.75	122.43
1	1	32	ARG	CA-C-N	-5.01	112.95	121.97
1	1	32	ARG	C-N-CA	-5.01	112.95	121.97
2	2	228	ALA	N-CA-C	5.01	117.56	109.40
1	1	28	GLU	O-C-N	5.01	129.25	122.59
1	1	74	PRO	CA-C-O	-5.00	115.88	121.23
1	1	163	PRO	N-CA-C	5.00	118.36	110.50
2	2	187	THR	O-C-N	5.00	129.37	122.46

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	1	2005	0	1952	111	0
2	2	1982	0	1871	108	0
3	3	1774	0	1730	98	0
4	4	192	0	171	16	0
5	1	121	0	0	8	0
5	2	108	0	0	13	0
5	3	88	0	0	4	0
5	4	10	0	0	0	0
All	All	6280	0	5724	306	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 26.

All (306) 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)
2:2:127:LEU:HB2	2:2:230:PHE:CZ	1.60	1.34
2:2:127:LEU:HB2	2:2:230:PHE:CE2	1.75	1.21
2:2:163:ALA:CB	3:3:232:GLN:HG3	1.73	1.16
2:2:141:LYS:HD3	2:2:144:ASP:OD2	1.45	1.16
2:2:163:ALA:HB2	3:3:232:GLN:HG3	1.16	1.14
1:1:22:GLU:HB2	1:1:23:PRO:HD2	1.33	1.08
2:2:141:LYS:O	2:2:141:LYS:HG2	1.59	1.01
2:2:183:GLN:H	2:2:183:GLN:HE21	1.06	1.00
2:2:127:LEU:CB	2:2:230:PHE:CZ	2.44	0.99
1:1:223:ARG:NH1	5:1:336:HOH:O	1.96	0.98
1:1:14:ASP:HB2	3:3:217:ASP:OD2	1.64	0.98
2:2:219:GLN:HB3	5:2:328:HOH:O	1.64	0.96
3:3:172:ARG:HD3	5:3:295:HOH:O	1.64	0.96
2:2:218:THR:HG23	5:2:328:HOH:O	1.66	0.94
1:1:154:VAL:O	1:1:154:VAL:HG12	1.65	0.94
1:1:68:LEU:HD12	1:1:68:LEU:C	1.95	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:58:ASN:O	3:3:61:ASN:HA	1.70	0.91
1:1:22:GLU:HB2	1:1:23:PRO:CD	2.00	0.91
2:2:127:LEU:HD22	2:2:230:PHE:HZ	1.38	0.89
2:2:138:LYS:NZ	2:2:152:THR:HG22	1.88	0.89
2:2:161:GLN:HE21	2:2:164:PRO:HA	1.34	0.89
2:2:218:THR:HB	5:2:354:HOH:O	1.72	0.88
3:3:61:ASN:O	3:3:61:ASN:ND2	2.07	0.87
1:1:50:GLN:NE2	1:1:57:VAL:H	1.72	0.87
2:2:161:GLN:HE22	2:2:166:GLY:H	1.23	0.87
2:2:264:VAL:HG12	2:2:264:VAL:O	1.75	0.86
2:2:127:LEU:CB	2:2:230:PHE:CE2	2.58	0.84
3:3:59:SER:C	3:3:61:ASN:H	1.85	0.83
2:2:141:LYS:CD	2:2:144:ASP:OD2	2.24	0.83
3:3:58:ASN:O	3:3:61:ASN:N	2.11	0.83
4:4:22:ILE:HG22	4:4:22:ILE:O	1.79	0.83
1:1:154:VAL:O	1:1:154:VAL:CG1	2.26	0.82
3:3:144:MET:O	3:3:144:MET:HG2	1.77	0.82
2:2:141:LYS:HD2	2:2:144:ASP:HB2	1.60	0.82
1:1:22:GLU:CB	1:1:23:PRO:HD2	2.08	0.82
1:1:59:GLN:H	1:1:66:ASN:HD21	1.30	0.80
3:3:74:PRO:HD2	3:3:192:GLN:HG3	1.61	0.80
4:4:20:VAL:O	4:4:23:ASN:HB3	1.83	0.79
1:1:11:SER:OG	1:1:13:ASP:OD1	2.00	0.78
2:2:138:LYS:HZ3	2:2:152:THR:HG22	1.47	0.76
3:3:144:MET:HE1	3:3:145:GLN:NE2	2.01	0.76
3:3:144:MET:CE	3:3:145:GLN:NE2	2.49	0.75
1:1:145:TRP:HE3	1:1:171:PRO:HG2	1.49	0.75
2:2:212:ALA:HB1	2:2:213:PRO:HD2	1.70	0.74
1:1:59:GLN:H	1:1:66:ASN:ND2	1.85	0.74
2:2:218:THR:CG2	5:2:328:HOH:O	2.30	0.74
2:2:163:ALA:CB	3:3:232:GLN:CG	2.61	0.73
3:3:58:ASN:O	3:3:61:ASN:CA	2.35	0.73
3:3:78:LEU:HD11	3:3:192:GLN:HG2	1.69	0.73
2:2:127:LEU:HD22	2:2:230:PHE:CZ	2.21	0.73
2:2:183:GLN:HE21	2:2:183:GLN:N	1.85	0.73
2:2:156:THR:HB	5:2:370:HOH:O	1.89	0.73
2:2:264:VAL:HA	5:2:345:HOH:O	1.88	0.73
4:4:24:ASN:O	4:4:26:TYR:N	2.22	0.73
3:3:61:ASN:O	3:3:61:ASN:CG	2.29	0.73
1:1:145:TRP:CE3	1:1:171:PRO:HG2	2.24	0.72
4:4:21:ILE:C	4:4:23:ASN:H	1.98	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:59:SER:C	3:3:61:ASN:N	2.47	0.71
3:3:185:ASP:OD2	5:3:304:HOH:O	2.08	0.71
1:1:14:ASP:C	1:1:14:ASP:OD1	2.33	0.71
3:3:61:ASN:C	3:3:61:ASN:HD22	1.98	0.71
3:3:84:ALA:HA	5:3:304:HOH:O	1.91	0.70
3:3:144:MET:HE2	3:3:145:GLN:CD	2.17	0.70
1:1:247:ARG:HB2	1:1:248:PRO:HD2	1.73	0.70
1:1:61:ASN:C	1:1:61:ASN:HD22	2.00	0.69
3:3:61:ASN:ND2	3:3:61:ASN:C	2.49	0.69
2:2:265:ILE:HG22	2:2:266:ALA:N	2.06	0.69
1:1:52:ILE:HG12	1:1:163:PRO:HG3	1.74	0.69
1:1:16:SER:HB3	1:1:22:GLU:HA	1.75	0.69
1:1:51:ASN:HB3	1:1:53:GLU:H	1.55	0.69
4:4:24:ASN:H	4:4:24:ASN:ND2	1.90	0.69
4:4:24:ASN:HD22	4:4:25:PHE:H	1.38	0.69
1:1:22:GLU:CB	1:1:23:PRO:CD	2.64	0.68
1:1:68:LEU:C	1:1:68:LEU:CD1	2.66	0.67
2:2:163:ALA:HB1	3:3:232:GLN:HG3	1.72	0.67
2:2:183:GLN:H	2:2:183:GLN:NE2	1.85	0.67
3:3:84:ALA:O	3:3:87:CYS:N	2.27	0.67
1:1:61:ASN:ND2	1:1:64:ARG:HH21	1.92	0.67
2:2:127:LEU:CD2	2:2:230:PHE:HZ	2.08	0.67
2:2:127:LEU:HD13	2:2:230:PHE:CE2	2.29	0.67
1:1:165:LEU:HD12	1:1:227:GLN:HB2	1.77	0.67
2:2:77:PHE:CE2	3:3:65:PRO:HG3	2.30	0.66
2:2:127:LEU:HD13	2:2:230:PHE:CZ	2.31	0.66
2:2:161:GLN:NE2	2:2:164:PRO:HA	2.08	0.65
3:3:136:LYS:HB2	3:3:187:TRP:CE2	2.30	0.65
2:2:77:PHE:O	2:2:79:HIS:HD2	1.79	0.65
3:3:84:ALA:O	3:3:87:CYS:HB3	1.98	0.64
3:3:18:ASN:HD22	3:3:19:PRO:CD	2.12	0.63
1:1:24:VAL:N	3:3:217:ASP:OD1	2.31	0.63
2:2:163:ALA:HB2	3:3:232:GLN:CG	2.11	0.63
1:1:118:SER:C	1:1:120:PHE:H	2.06	0.63
3:3:144:MET:CE	3:3:145:GLN:CD	2.72	0.63
3:3:18:ASN:HD22	3:3:19:PRO:N	1.96	0.62
3:3:82:GLN:NE2	3:3:184:VAL:HG11	2.14	0.62
3:3:45:LEU:O	3:3:48:CYS:HB2	1.98	0.62
2:2:146:GLU:HB3	2:2:147:PRO:HD2	1.80	0.62
2:2:127:LEU:CG	2:2:230:PHE:CZ	2.82	0.62
3:3:18:ASN:HD22	3:3:19:PRO:HD2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:162:THR:O	3:3:164:PRO:HD3	1.99	0.62
3:3:43:ASP:O	3:3:46:GLU:HG3	1.99	0.61
3:3:88:SER:O	3:3:91:CYS:HB2	2.01	0.61
1:1:51:ASN:HB2	1:1:54:SER:OG	2.02	0.60
3:3:136:LYS:HG3	3:3:137:PRO:HD2	1.84	0.60
3:3:18:ASN:ND2	3:3:19:PRO:HD2	2.17	0.59
1:1:56:PHE:CD1	1:1:56:PHE:C	2.81	0.59
1:1:119:PRO:HB2	3:3:47:LEU:HD13	1.85	0.58
1:1:145:TRP:CG	1:1:146:ALA:N	2.72	0.58
2:2:181:GLN:CG	2:2:186:TRP:HE1	2.18	0.57
1:1:162:THR:HB	1:1:163:PRO:HD2	1.87	0.56
2:2:102:ARG:NH2	5:2:352:HOH:O	2.24	0.56
1:1:3:ASP:OD1	1:1:4:ASN:N	2.27	0.56
1:1:54:SER:O	1:1:227:GLN:NE2	2.38	0.56
1:1:6:GLU:HA	2:2:193:ILE:HB	1.88	0.56
1:1:255:PRO:HG3	3:3:88:SER:HB2	1.87	0.56
2:2:264:VAL:CA	5:2:345:HOH:O	2.51	0.56
3:3:64:TYR:C	3:3:66:TYR:H	2.12	0.56
2:2:163:ALA:HB1	3:3:232:GLN:CG	2.32	0.55
2:2:165:THR:HG22	3:3:231:PRO:HB2	1.88	0.55
3:3:108:SER:OG	3:3:217:ASP:OD2	2.25	0.55
1:1:119:PRO:CB	3:3:47:LEU:HD13	2.36	0.55
4:4:24:ASN:O	4:4:26:TYR:O	2.25	0.55
1:1:128:GLU:HB3	1:1:237:ARG:HB3	1.88	0.55
3:3:172:ARG:CZ	3:3:185:ASP:HB3	2.37	0.55
1:1:101:THR:HG22	1:1:102:THR:N	2.21	0.55
2:2:67:LEU:HB2	2:2:245:ILE:O	2.07	0.55
1:1:23:PRO:HA	3:3:217:ASP:OD1	2.06	0.54
1:1:117:PHE:CE1	1:1:119:PRO:HG3	2.43	0.54
2:2:127:LEU:CD2	2:2:230:PHE:CZ	2.88	0.54
3:3:84:ALA:O	3:3:87:CYS:CB	2.55	0.54
1:1:247:ARG:NH2	5:1:308:HOH:O	2.40	0.54
3:3:88:SER:HA	5:3:316:HOH:O	2.08	0.54
2:2:138:LYS:NZ	2:2:149:ASP:O	2.41	0.54
3:3:83:VAL:HG21	3:3:129:TYR:CE1	2.43	0.54
3:3:74:PRO:HG2	3:3:78:LEU:HD21	1.90	0.53
1:1:76:PHE:O	1:1:77:CYS:C	2.52	0.53
3:3:18:ASN:HD22	3:3:18:ASN:C	2.17	0.53
1:1:250:LEU:HD21	3:3:231:PRO:HG3	1.91	0.53
2:2:217:TRP:CG	2:2:218:THR:N	2.77	0.52
2:2:261:HIS:HD2	5:2:279:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:90:MET:O	3:3:92:ASN:N	2.43	0.52
3:3:3:ILE:N	3:3:3:ILE:CD1	2.73	0.52
3:3:106:ARG:HH12	3:3:170:HIS:HD2	1.57	0.52
1:1:114:PHE:CD1	1:1:114:PHE:C	2.88	0.52
1:1:42:PRO:HA	1:1:235:ARG:HB3	1.91	0.52
1:1:201:PHE:O	1:1:203:GLY:N	2.39	0.52
3:3:20:ASP:OD1	3:3:21:THR:N	2.40	0.52
2:2:141:LYS:CD	2:2:144:ASP:HB2	2.37	0.51
3:3:62:LYS:HD3	3:3:64:TYR:OH	2.10	0.51
1:1:32:ARG:O	1:1:33:VAL:C	2.53	0.51
1:1:80:SER:C	1:1:82:SER:N	2.68	0.51
3:3:66:TYR:HB3	3:3:209:LEU:HA	1.91	0.51
3:3:70:THR:OG1	3:3:71:ASN:N	2.41	0.51
2:2:218:THR:CG2	2:2:219:GLN:N	2.73	0.51
1:1:42:PRO:HG3	1:1:235:ARG:NH1	2.26	0.50
1:1:223:ARG:NE	5:1:351:HOH:O	2.19	0.50
1:1:244:PHE:CD1	1:1:244:PHE:N	2.80	0.50
3:3:9:GLU:HG2	3:3:10:HIS:N	2.26	0.50
1:1:240:LYS:O	1:1:240:LYS:HG3	2.11	0.50
1:1:244:PHE:CD2	3:3:40:GLU:HB2	2.45	0.50
1:1:119:PRO:HB2	3:3:47:LEU:CD1	2.41	0.50
1:1:76:PHE:CG	1:1:77:CYS:N	2.79	0.50
2:2:127:LEU:CD1	2:2:230:PHE:CE2	2.94	0.50
4:4:21:ILE:O	4:4:23:ASN:N	2.42	0.50
2:2:33:LEU:HD13	2:2:33:LEU:C	2.37	0.50
2:2:40:HIS:O	2:2:253:ASN:ND2	2.37	0.50
2:2:33:LEU:HB3	2:2:204:LEU:HD23	1.94	0.50
4:4:17:ASN:CG	4:4:17:ASN:O	2.55	0.49
1:1:247:ARG:HB2	1:1:248:PRO:CD	2.39	0.49
3:3:136:LYS:HD2	3:3:187:TRP:CD1	2.47	0.49
1:1:61:ASN:C	1:1:61:ASN:ND2	2.64	0.49
2:2:25:ASN:ND2	5:2:348:HOH:O	2.38	0.49
2:2:127:LEU:CD1	2:2:230:PHE:CZ	2.96	0.49
3:3:59:SER:O	3:3:61:ASN:N	2.44	0.49
1:1:118:SER:O	1:1:120:PHE:N	2.44	0.49
2:2:264:VAL:C	5:2:345:HOH:O	2.55	0.49
3:3:49:LYS:O	3:3:51:PRO:HD3	2.12	0.49
4:4:23:ASN:CG	4:4:23:ASN:O	2.51	0.49
3:3:90:MET:O	3:3:91:CYS:C	2.56	0.49
4:4:29:GLN:HG3	4:4:34:ILE:HD11	1.94	0.49
2:2:251:PRO:HB2	2:2:254:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:31:SER:HB2	4:4:33:SER:HB2	1.95	0.49
3:3:18:ASN:C	3:3:20:ASP:H	2.19	0.48
3:3:106:ARG:HH12	3:3:170:HIS:CD2	2.31	0.48
1:1:109:LYS:O	1:1:110:GLN:HB3	2.13	0.48
2:2:138:LYS:CE	2:2:152:THR:HG22	2.42	0.48
1:1:3:ASP:CG	1:1:4:ASN:H	2.12	0.48
1:1:137:ASP:O	1:1:138:THR:C	2.55	0.48
2:2:260:ARG:HH11	2:2:260:ARG:HG3	1.78	0.48
1:1:68:LEU:HB2	5:1:362:HOH:O	2.14	0.48
1:1:200:TRP:CH2	1:1:214:GLY:HA3	2.49	0.48
2:2:181:GLN:HG3	2:2:186:TRP:HE1	1.78	0.48
2:2:17:ASP:OD2	2:2:62:TYR:OH	2.27	0.48
3:3:198:TYR:HB2	3:3:199:PRO:HD2	1.95	0.48
4:4:31:GLN:O	4:4:31:GLN:HG3	2.13	0.48
1:1:125:CYS:HB3	1:1:241:MET:HA	1.96	0.47
2:2:132:PRO:HD3	2:2:223:TRP:CZ3	2.49	0.47
2:2:181:GLN:HG2	2:2:186:TRP:HE1	1.79	0.47
1:1:68:LEU:HD12	1:1:68:LEU:O	2.12	0.47
1:1:68:LEU:O	1:1:223:ARG:HB2	2.15	0.47
1:1:60:GLU:HG2	1:1:61:ASN:N	2.28	0.47
3:3:82:GLN:O	3:3:84:ALA:N	2.48	0.47
2:2:127:LEU:CG	2:2:230:PHE:HZ	2.26	0.47
2:2:163:ALA:O	2:2:165:THR:N	2.46	0.47
3:3:43:ASP:OD1	3:3:45:LEU:HB2	2.15	0.47
2:2:32:ARG:HH21	2:2:111:ARG:HD3	1.79	0.47
4:4:22:ILE:O	4:4:24:ASN:ND2	2.48	0.47
2:2:102:ARG:HG2	2:2:262:GLU:HB2	1.96	0.47
1:1:60:GLU:HG2	1:1:61:ASN:H	1.79	0.46
1:1:74:PRO:HA	1:1:110:GLN:HB3	1.97	0.46
3:3:82:GLN:CD	3:3:184:VAL:HG11	2.40	0.46
2:2:35:GLY:C	2:2:37:GLY:N	2.72	0.46
2:2:123:ALA:HB3	2:2:234:GLN:HB2	1.97	0.46
1:1:66:ASN:ND2	5:1:378:HOH:O	2.48	0.46
2:2:56:VAL:O	2:2:60:GLU:HG3	2.14	0.46
2:2:144:ASP:O	2:2:145:MET:HB2	2.14	0.46
2:2:146:GLU:HB3	2:2:147:PRO:CD	2.46	0.46
1:1:255:PRO:CG	3:3:88:SER:HB2	2.46	0.46
2:2:88:LEU:O	2:2:93:GLY:HA3	2.16	0.46
2:2:265:ILE:O	2:2:266:ALA:C	2.59	0.46
1:1:85:VAL:HG12	1:1:88:LYS:HG3	1.97	0.46
3:3:64:TYR:C	3:3:66:TYR:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:144:MET:HE2	3:3:145:GLN:NE2	2.25	0.46
2:2:199:ASN:N	2:2:199:ASN:OD1	2.49	0.45
1:1:153:ASP:O	1:1:153:ASP:CG	2.56	0.45
1:1:8:GLY:O	1:1:9:LYS:HB3	2.16	0.45
2:2:84:LEU:HB3	2:2:110:TRP:CZ2	2.51	0.45
2:2:161:GLN:HE22	2:2:166:GLY:N	2.03	0.45
1:1:33:VAL:HG11	1:1:243:VAL:HG22	1.99	0.45
2:2:149:ASP:N	2:2:150:PRO:CD	2.80	0.45
1:1:60:GLU:CG	1:1:61:ASN:N	2.80	0.45
1:1:223:ARG:NH2	5:1:351:HOH:O	2.50	0.45
1:1:25:LYS:HG3	1:1:26:LEU:N	2.32	0.44
1:1:66:ASN:N	1:1:66:ASN:HD22	2.16	0.44
2:2:171:SER:HA	5:2:367:HOH:O	2.18	0.44
1:1:188:PRO:O	1:1:190:ASN:N	2.50	0.44
1:1:153:ASP:C	1:1:155:THR:H	2.26	0.44
3:3:31:SER:O	3:3:32:THR:C	2.59	0.44
3:3:138:THR:C	3:3:139:THR:CG2	2.91	0.44
1:1:14:ASP:HB3	3:3:216:ASP:HB3	1.99	0.44
2:2:169:TYR:C	2:2:171:SER:H	2.26	0.44
3:3:91:CYS:O	3:3:100:ARG:NH2	2.50	0.44
2:2:127:LEU:HD13	2:2:230:PHE:HE2	1.79	0.43
3:3:15:TYR:HB2	3:3:18:ASN:HB2	1.99	0.43
1:1:254:TRP:CH2	3:3:55:GLY:HA3	2.53	0.43
2:2:209:VAL:O	2:2:210:ASN:HB2	2.17	0.43
2:2:144:ASP:O	2:2:145:MET:CB	2.66	0.43
3:3:58:ASN:C	3:3:61:ASN:H	2.25	0.43
1:1:51:ASN:O	1:1:227:GLN:HG2	2.19	0.43
1:1:117:PHE:CZ	1:1:119:PRO:HG3	2.53	0.43
2:2:19:ALA:HB1	2:2:61:ARG:HA	2.00	0.43
2:2:86:HIS:H	2:2:86:HIS:CD2	2.36	0.43
1:1:76:PHE:HB3	1:1:93:TRP:CE2	2.53	0.43
2:2:164:PRO:HG3	2:2:183:GLN:NE2	2.34	0.43
2:2:78:SER:HA	2:2:160:PRO:HD3	2.01	0.43
2:2:217:TRP:CD2	2:2:218:THR:N	2.87	0.43
3:3:40:GLU:CG	3:3:41:PHE:N	2.79	0.43
1:1:252:PHE:CG	1:1:253:PRO:HD2	2.54	0.43
1:1:213:PHE:CZ	2:2:150:PRO:HB3	2.54	0.43
1:1:185:PHE:HA	3:3:22:THR:HG23	2.01	0.42
3:3:84:ALA:O	3:3:85:LEU:C	2.61	0.42
3:3:90:MET:C	3:3:92:ASN:N	2.77	0.42
1:1:66:ASN:HD22	1:1:66:ASN:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:ARG:NH2	2:2:111:ARG:HD3	2.35	0.42
4:4:23:ASN:N	4:4:23:ASN:HD22	2.17	0.42
1:1:170:ASN:HB3	1:1:171:PRO:HD2	2.01	0.42
1:1:223:ARG:CZ	5:1:351:HOH:O	2.64	0.42
1:1:245:CYS:HB3	2:2:36:TYR:OH	2.19	0.42
1:1:252:PHE:HA	1:1:253:PRO:HD3	1.91	0.42
1:1:254:TRP:HZ2	2:2:184:TRP:CE2	2.38	0.42
2:2:149:ASP:N	2:2:150:PRO:HD3	2.35	0.42
1:1:80:SER:O	1:1:82:SER:N	2.53	0.42
3:3:11:LYS:C	3:3:13:CYS:H	2.27	0.42
3:3:198:TYR:HB2	3:3:199:PRO:CD	2.50	0.42
1:1:125:CYS:HB2	1:1:239:LYS:O	2.20	0.42
4:4:25:PHE:HB3	4:4:26:TYR:H	1.74	0.42
1:1:216:ALA:HA	1:1:217:PRO:HD3	1.88	0.41
1:1:248:PRO:HB3	2:2:185:GLN:HB2	2.01	0.41
2:2:138:LYS:HE2	2:2:152:THR:CG2	2.50	0.41
1:1:104:PHE:HA	1:1:105:PRO:C	2.45	0.41
1:1:152:ALA:C	1:1:154:VAL:N	2.78	0.41
2:2:127:LEU:HD13	2:2:230:PHE:HZ	1.83	0.41
3:3:139:THR:O	3:3:140:ARG:C	2.63	0.41
1:1:68:LEU:HD12	1:1:69:LEU:N	2.32	0.41
1:1:80:SER:O	1:1:81:THR:C	2.62	0.41
2:2:191:HIS:CD2	2:2:191:HIS:C	2.98	0.41
3:3:121:VAL:HG12	3:3:122:LYS:N	2.34	0.41
1:1:3:ASP:HB2	5:1:338:HOH:O	2.20	0.41
2:2:265:ILE:N	5:2:345:HOH:O	2.54	0.41
3:3:73:VAL:HA	3:3:74:PRO:HD2	1.91	0.41
1:1:245:CYS:HA	1:1:246:PRO:HD2	1.85	0.41
2:2:32:ARG:CZ	2:2:111:ARG:NH1	2.84	0.41
2:2:134:PHE:CE1	2:2:181:GLN:HG2	2.56	0.41
2:2:218:THR:HG22	2:2:219:GLN:N	2.36	0.41
3:3:121:VAL:CG1	3:3:122:LYS:N	2.84	0.41
1:1:104:PHE:HB3	1:1:105:PRO:HA	2.03	0.40
1:1:187:VAL:HA	1:1:188:PRO:HD3	1.85	0.40
2:2:181:GLN:HE21	2:2:181:GLN:HB2	1.70	0.40
3:3:187:TRP:N	3:3:187:TRP:CE3	2.89	0.40
2:2:35:GLY:C	2:2:37:GLY:H	2.29	0.40
2:2:141:LYS:HD3	2:2:144:ASP:CG	2.38	0.40
2:2:151:PHE:CD1	2:2:151:PHE:N	2.85	0.40
1:1:118:SER:C	1:1:120:PHE:N	2.76	0.40
1:1:226:ILE:HG12	1:1:227:GLN:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:58:TYR:HA	1:1:66:ASN:HD21	1.87	0.40
1:1:75:SER:HB2	1:1:91:VAL:O	2.21	0.40
3:3:36:TYR:CE2	3:3:37:MET:HG2	2.57	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	1	254/274 (93%)	222 (87%)	22 (9%)	10 (4%)	2	8
2	2	253/267 (95%)	221 (87%)	29 (12%)	3 (1%)	10	34
3	3	226/236 (96%)	197 (87%)	23 (10%)	6 (3%)	4	15
4	4	23/71 (32%)	16 (70%)	4 (17%)	3 (13%)	0	0
All	All	756/848 (89%)	656 (87%)	78 (10%)	22 (3%)	3	13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	51	ASN
1	1	202	ASN
3	3	83	VAL
3	3	91	CYS
4	4	22	ILE
4	4	25	PHE
1	1	119	PRO
3	3	60	ASN
3	3	87	CYS
4	4	23	ASN
1	1	33	VAL
1	1	81	THR

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Mol	Chain	Res	Type
1	1	189	TYR
2	2	86	HIS
2	2	164	PRO
2	2	218	THR
1	1	28	GLU
1	1	20	VAL
1	1	154	VAL
3	3	19	PRO
3	3	85	LEU
1	1	255	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	1	220/237 (93%)	205 (93%)	15 (7%)	14	42
2	2	211/223 (95%)	197 (93%)	14 (7%)	15	43
3	3	200/205 (98%)	187 (94%)	13 (6%)	15	43
4	4	22/53 (42%)	19 (86%)	3 (14%)	3	13
All	All	653/718 (91%)	608 (93%)	45 (7%)	14	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	51	ASN
1	1	54	SER
1	1	61	ASN
1	1	66	ASN
1	1	68	LEU
1	1	80	SER
1	1	82	SER
1	1	101	THR
1	1	118	SER
1	1	154	VAL
1	1	158	LEU

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Mol	Chain	Res	Type
1	1	173	MET
1	1	212	ASP
1	1	242	LYS
1	1	247	ARG
2	2	12	ASP
2	2	69	SER
2	2	141	LYS
2	2	145	MET
2	2	152	THR
2	2	153	MET
2	2	171	SER
2	2	181	GLN
2	2	183	GLN
2	2	195	ASN
2	2	197	ARG
2	2	218	THR
2	2	263	THR
2	2	265	ILE
3	3	1	SER
3	3	3	ILE
3	3	30	ILE
3	3	35	ASP
3	3	42	SER
3	3	59	SER
3	3	75	THR
3	3	88	SER
3	3	91	CYS
3	3	108	SER
3	3	144	MET
3	3	158	SER
3	3	192	GLN
4	4	23	ASN
4	4	24	ASN
4	4	27	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	50	GLN
1	1	61	ASN
1	1	66	ASN
1	1	92	GLN

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Mol	Chain	Res	Type
1	1	103	ASN
1	1	170	ASN
1	1	218	ASN
2	2	25	ASN
2	2	79	HIS
2	2	86	HIS
2	2	161	GLN
2	2	181	GLN
2	2	183	GLN
2	2	195	ASN
2	2	244	GLN
2	2	261	HIS
3	3	10	HIS
3	3	18	ASN
3	3	60	ASN
3	3	61	ASN
3	3	71	ASN
3	3	82	GLN
3	3	170	HIS
3	3	205	ASN
4	4	23	ASN
4	4	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	7
2	2	4
3	3	3
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	226:ILE	C	227:GLN	N	1.20
1	1	251:PHE	C	252:PHE	N	1.20
1	2	146:GLU	C	147:PRO	N	1.20
1	3	79:VAL	C	80:ASP	N	1.20
1	3	215:GLY	C	216:ASP	N	1.20
1	1	60:GLU	C	61:ASN	N	1.19
1	1	126:ASP	C	127:LEU	N	1.19
1	2	24:THR	C	25:ASN	N	1.19
1	2	160:PRO	C	161:GLN	N	1.19
1	3	109:LEU	C	110:ASN	N	1.19
1	4	35:ASP	C	36:LEU	N	1.19
1	1	184:SER	C	185:PHE	N	1.18
1	1	90:PRO	C	91:VAL	N	1.17
1	2	254:PRO	C	255:VAL	N	1.17
1	1	27:PRO	C	28:GLU	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.