



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:20 PM UTC

PDB ID : 1GN4 / pdb_00001gn4
Title : H145E mutant of Mycobacterium tuberculosis iron-superoxide dismutase.
Authors : Bunting, K.A.; Cooper, J.B.; Badasso, M.O.; Tickle, I.J.; Newton, M.; Wood, S.P.; Zhang, Y.; Young, D.B.
Deposited on : 2001-10-02
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

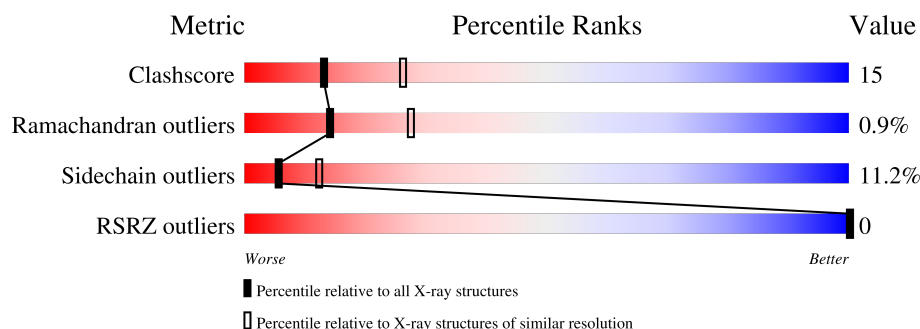
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	207	
1	B	207	
1	C	207	
1	D	207	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6560 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 SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			
1	B	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			
1	C	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			
1	D	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	81	Total	O	0	0
			81	81		
3	C	69	Total	O	0	0
			69	69		
3	D	68	Total	O	0	0
			68	68		

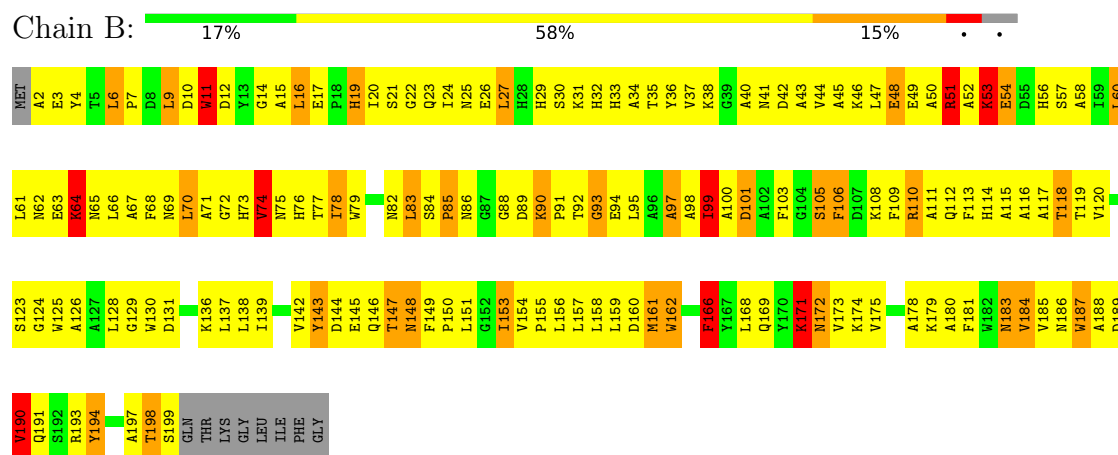
3 Residue-property plots

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

• Molecule 1: SUPEROXIDE DISMUTASE



• Molecule 1: SUPEROXIDE DISMUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.66Å 102.86Å 73.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.50) 94.1 (20.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.50Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.172 , 0.225 0.153 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.59	123/1615 (7.6%)	2.86	204/2203 (9.3%)
1	B	2.66	121/1615 (7.5%)	2.94	230/2203 (10.4%)
1	C	2.63	123/1615 (7.6%)	2.93	207/2203 (9.4%)
1	D	2.42	106/1615 (6.6%)	2.86	206/2203 (9.4%)
All	All	2.58	473/6460 (7.3%)	2.90	847/8812 (9.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	0
1	D	1	0
All	All	3	0

All (473) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	PHE	N-CA	16.26	1.66	1.46
1	C	55	ASP	N-CA	16.00	1.65	1.46
1	D	141	GLN	N-CA	15.02	1.64	1.46
1	A	175	VAL	N-CA	15.00	1.66	1.46
1	A	114	HIS	N-CA	14.95	1.66	1.46
1	C	149	PHE	N-CA	14.35	1.58	1.46
1	C	154	VAL	N-CA	14.04	1.61	1.46
1	B	76	HIS	N-CA	13.72	1.64	1.46
1	C	40	ALA	N-CA	13.62	1.63	1.46
1	B	63	GLU	N-CA	13.32	1.62	1.46
1	B	47	LEU	N-CA	13.17	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	ALA	N-CA	12.97	1.62	1.46
1	A	157	LEU	N-CA	12.80	1.61	1.45
1	A	126	ALA	N-CA	12.79	1.61	1.45
1	A	37	VAL	N-CA	12.56	1.61	1.46
1	C	83	LEU	N-CA	12.44	1.61	1.45
1	D	117	ALA	CA-CB	12.32	1.74	1.53
1	B	44	VAL	N-CA	12.25	1.61	1.46
1	B	46	LYS	N-CA	12.21	1.62	1.46
1	C	172	ASN	N-CA	12.17	1.63	1.46
1	D	83	LEU	N-CA	12.12	1.60	1.45
1	C	150	PRO	CA-CB	12.12	1.73	1.54
1	B	12	ASP	N-CA	12.05	1.61	1.45
1	B	67	ALA	N-CA	12.04	1.61	1.46
1	A	154	VAL	N-CA	11.94	1.55	1.46
1	D	169	GLN	N-CA	11.90	1.61	1.46
1	B	79	TRP	N-CA	11.67	1.61	1.46
1	B	40	ALA	N-CA	11.63	1.60	1.46
1	C	157	LEU	N-CA	11.61	1.60	1.46
1	C	70	LEU	N-CA	11.59	1.60	1.46
1	B	142	VAL	N-CA	11.58	1.59	1.46
1	B	68	PHE	N-CA	11.50	1.60	1.46
1	D	61	LEU	N-CA	11.46	1.60	1.46
1	D	177	PHE	N-CA	11.45	1.60	1.46
1	B	154	VAL	N-CA	11.38	1.56	1.46
1	A	109	PHE	N-CA	11.21	1.59	1.46
1	C	194	TYR	N-CA	11.19	1.60	1.46
1	D	111	ALA	N-CA	11.07	1.60	1.46
1	D	121	GLN	N-CA	11.06	1.61	1.46
1	C	165	ALA	N-CA	10.97	1.60	1.46
1	B	70	LEU	N-CA	10.87	1.59	1.46
1	B	169	GLN	N-CA	10.86	1.59	1.46
1	A	63	GLU	N-CA	10.84	1.60	1.46
1	A	38	LYS	N-CA	10.82	1.59	1.46
1	C	120	VAL	CA-CB	10.78	1.68	1.54
1	D	131	ASP	CA-CB	10.72	1.67	1.53
1	B	74	VAL	N-CA	10.69	1.59	1.46
1	C	186	ASN	N-CA	10.68	1.61	1.46
1	D	79	TRP	N-CA	10.67	1.59	1.46
1	B	78	ILE	N-CA	10.63	1.60	1.46
1	B	27	LEU	N-CA	10.61	1.59	1.46
1	A	115	ALA	N-CA	10.60	1.59	1.46
1	D	35	THR	N-CA	10.54	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	TYR	N-CA	10.51	1.58	1.46
1	B	35	THR	N-CA	10.50	1.59	1.46
1	A	97	ALA	N-CA	10.47	1.59	1.46
1	C	114	HIS	N-CA	10.46	1.59	1.46
1	B	41	ASN	N-CA	10.45	1.59	1.46
1	C	48	GLU	N-CA	10.34	1.58	1.46
1	C	126	ALA	N-CA	10.27	1.58	1.46
1	C	3	GLU	N-CA	10.20	1.58	1.45
1	D	36	TYR	N-CA	10.07	1.58	1.46
1	B	64	LYS	N-CA	10.05	1.58	1.46
1	A	193	ARG	N-CA	10.03	1.59	1.46
1	D	159	LEU	N-CA	10.02	1.58	1.46
1	C	58	ALA	N-CA	10.01	1.57	1.46
1	B	50	ALA	N-CA	10.00	1.59	1.46
1	B	115	ALA	N-CA	9.96	1.58	1.46
1	C	63	GLU	N-CA	9.95	1.59	1.46
1	C	73	HIS	N-CA	9.95	1.59	1.46
1	C	162	TRP	N-CA	9.93	1.58	1.46
1	A	149	PHE	N-CA	9.88	1.55	1.46
1	B	38	LYS	N-CA	9.82	1.59	1.46
1	B	190	VAL	N-CA	9.80	1.58	1.46
1	D	46	LYS	N-CA	9.75	1.58	1.46
1	A	138	LEU	N-CA	9.74	1.58	1.46
1	D	157	LEU	N-CA	9.74	1.58	1.46
1	B	145	GLU	N-CA	9.71	1.59	1.46
1	A	195	ALA	N-CA	9.71	1.58	1.46
1	B	162	TRP	N-CA	9.65	1.58	1.45
1	D	37	VAL	CA-CB	9.63	1.67	1.54
1	B	37	VAL	N-CA	9.63	1.57	1.46
1	C	101	ASP	CA-CB	9.61	1.69	1.53
1	B	46	LYS	CA-CB	9.56	1.70	1.53
1	B	73	HIS	N-CA	9.54	1.57	1.46
1	C	180	ALA	N-CA	9.52	1.58	1.46
1	B	40	ALA	CA-CB	9.46	1.68	1.53
1	D	23	GLN	N-CA	9.44	1.57	1.46
1	A	92	THR	CA-CB	9.43	1.70	1.53
1	D	4	TYR	N-CA	9.41	1.57	1.45
1	C	159	LEU	N-CA	9.36	1.57	1.46
1	A	26	GLU	N-CA	9.36	1.58	1.46
1	B	71	ALA	N-CA	9.28	1.57	1.46
1	A	31	LYS	N-CA	9.24	1.58	1.46
1	D	43	ALA	N-CA	9.22	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	THR	N-CA	9.21	1.57	1.45
1	D	25	ASN	N-CA	9.21	1.57	1.46
1	D	33	HIS	N-CA	9.21	1.57	1.46
1	A	66	LEU	N-CA	9.20	1.57	1.46
1	C	109	PHE	N-CA	9.19	1.57	1.46
1	C	47	LEU	N-CA	9.17	1.58	1.46
1	C	27	LEU	N-CA	9.17	1.57	1.46
1	B	139	ILE	N-CA	9.16	1.57	1.46
1	C	140	PHE	N-CA	9.16	1.57	1.45
1	A	74	VAL	CA-CB	9.12	1.67	1.54
1	C	142	VAL	CA-CB	9.12	1.66	1.54
1	C	138	LEU	N-CA	9.10	1.57	1.45
1	D	58	ALA	N-CA	9.03	1.56	1.46
1	A	153	ILE	CA-CB	9.01	1.66	1.54
1	A	111	ALA	N-CA	8.96	1.57	1.46
1	C	198	THR	CB-OG1	8.89	1.57	1.43
1	B	60	LEU	CA-CB	8.88	1.67	1.53
1	C	37	VAL	N-CA	8.86	1.56	1.46
1	B	157	LEU	N-CA	8.85	1.57	1.46
1	A	166	PHE	N-CA	8.84	1.57	1.46
1	B	23	GLN	N-CA	8.83	1.57	1.46
1	B	43	ALA	N-CA	8.82	1.57	1.46
1	B	49	GLU	N-CA	8.81	1.57	1.46
1	B	20	ILE	N-CA	8.80	1.57	1.46
1	B	58	ALA	N-CA	8.78	1.56	1.46
1	D	4	TYR	CA-CB	8.78	1.67	1.53
1	D	73	HIS	N-CA	8.78	1.57	1.46
1	B	44	VAL	CA-CB	8.68	1.65	1.54
1	B	153	ILE	N-CA	8.64	1.56	1.46
1	A	35	THR	N-CA	8.62	1.56	1.46
1	C	34	ALA	N-CA	8.61	1.57	1.46
1	A	109	PHE	CA-CB	8.60	1.66	1.53
1	B	75	ASN	N-CA	8.59	1.57	1.46
1	C	116	ALA	N-CA	8.57	1.57	1.46
1	B	60	LEU	N-CA	8.55	1.56	1.46
1	C	42	ASP	N-CA	8.53	1.57	1.46
1	B	9	LEU	N-CA	8.53	1.56	1.45
1	C	26	GLU	N-CA	8.53	1.57	1.46
1	B	24	ILE	N-CA	8.51	1.56	1.46
1	C	77	THR	CA-CB	8.51	1.67	1.53
1	C	66	LEU	N-CA	8.47	1.56	1.46
1	B	179	LYS	N-CA	8.44	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	ASN	N-CA	8.42	1.57	1.46
1	A	73	HIS	N-CA	8.41	1.56	1.46
1	C	185	VAL	CA-CB	8.36	1.63	1.54
1	D	63	GLU	N-CA	8.34	1.57	1.46
1	D	149	PHE	N-CA	8.29	1.54	1.46
1	C	16	LEU	N-CA	8.29	1.56	1.46
1	B	62	ASN	N-CA	8.28	1.56	1.46
1	A	70	LEU	N-CA	8.25	1.56	1.46
1	D	29	HIS	N-CA	8.25	1.56	1.46
1	A	74	VAL	N-CA	8.24	1.57	1.46
1	A	139	ILE	N-CA	8.24	1.56	1.46
1	B	143	TYR	N-CA	8.22	1.55	1.46
1	B	51	ARG	N-CA	8.21	1.56	1.46
1	D	181	PHE	N-CA	8.20	1.56	1.46
1	D	114	HIS	N-CA	8.19	1.56	1.46
1	C	74	VAL	N-CA	8.18	1.56	1.46
1	A	151	LEU	CA-CB	8.16	1.66	1.53
1	A	3	GLU	CA-CB	8.14	1.65	1.53
1	A	175	VAL	CA-CB	8.14	1.64	1.54
1	D	145	GLU	N-CA	8.14	1.56	1.46
1	D	191	GLN	N-CA	8.13	1.56	1.46
1	B	120	VAL	CA-CB	8.12	1.64	1.54
1	A	161	MET	CA-CB	-8.09	1.40	1.53
1	D	17	GLU	N-CA	8.06	1.57	1.45
1	A	12	ASP	N-CA	8.06	1.55	1.45
1	B	42	ASP	N-CA	8.04	1.56	1.46
1	A	180	ALA	CA-CB	8.04	1.66	1.53
1	A	30	SER	CA-CB	8.03	1.67	1.53
1	C	62	ASN	N-CA	8.01	1.56	1.46
1	B	147	THR	N-CA	8.00	1.55	1.45
1	A	52	ALA	N-CA	7.97	1.56	1.46
1	B	66	LEU	N-CA	7.95	1.56	1.46
1	B	166	PHE	N-CA	7.92	1.56	1.46
1	A	186	ASN	N-CA	7.92	1.57	1.46
1	C	179	LYS	CA-CB	7.91	1.66	1.53
1	C	143	TYR	CA-CB	-7.90	1.42	1.53
1	C	179	LYS	N-CA	7.87	1.56	1.46
1	A	151	LEU	N-CA	7.86	1.56	1.45
1	B	34	ALA	N-CA	7.86	1.56	1.46
1	C	35	THR	N-CA	7.85	1.56	1.46
1	A	170	TYR	N-CA	7.85	1.56	1.45
1	C	139	ILE	N-CA	7.85	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	TYR	N-CA	7.84	1.55	1.46
1	A	145	GLU	N-CA	7.83	1.56	1.46
1	A	141	GLN	N-CA	7.81	1.55	1.46
1	D	8	ASP	N-CA	7.79	1.54	1.45
1	B	126	ALA	N-CA	7.78	1.55	1.46
1	A	45	ALA	N-CA	7.76	1.56	1.46
1	C	131	ASP	CA-CB	7.75	1.62	1.53
1	A	61	LEU	N-CA	7.75	1.56	1.46
1	D	126	ALA	CA-CB	-7.73	1.41	1.53
1	B	142	VAL	CA-CB	7.68	1.64	1.54
1	C	43	ALA	N-CA	7.68	1.55	1.46
1	B	114	HIS	N-CA	7.66	1.56	1.46
1	B	4	TYR	N-CA	7.58	1.55	1.45
1	D	150	PRO	CA-CB	7.58	1.64	1.54
1	C	193	ARG	N-CA	7.58	1.56	1.46
1	C	80	TRP	N-CA	7.57	1.55	1.46
1	B	190	VAL	CA-CB	-7.57	1.44	1.54
1	D	47	LEU	N-CA	7.56	1.55	1.46
1	A	40	ALA	CA-CB	7.56	1.65	1.53
1	D	146	GLN	N-CA	7.56	1.55	1.46
1	C	9	LEU	N-CA	7.55	1.54	1.45
1	C	50	ALA	N-CA	7.55	1.55	1.46
1	A	196	ALA	CA-CB	7.54	1.65	1.53
1	A	27	LEU	N-CA	7.53	1.56	1.46
1	B	86	ASN	CA-CB	7.51	1.65	1.53
1	B	68	PHE	CA-C	-7.49	1.43	1.52
1	A	35	THR	CB-OG1	7.42	1.55	1.43
1	B	158	LEU	N-CA	7.41	1.55	1.45
1	C	128	LEU	N-CA	7.40	1.55	1.46
1	B	99	ILE	CA-CB	7.39	1.62	1.54
1	D	74	VAL	N-CA	7.39	1.55	1.46
1	D	147	THR	N-CA	7.36	1.55	1.45
1	C	145	GLU	N-CA	7.35	1.56	1.45
1	C	141	GLN	CA-CB	7.34	1.63	1.53
1	D	188	ALA	N-CA	7.34	1.55	1.46
1	C	184	VAL	N-CA	7.33	1.55	1.46
1	B	153	ILE	CA-CB	7.33	1.62	1.54
1	C	146	GLN	CA-CB	7.32	1.64	1.53
1	C	127	ALA	N-CA	7.29	1.55	1.46
1	A	197	ALA	N-CA	7.28	1.55	1.46
1	B	48	GLU	N-CA	7.28	1.55	1.46
1	C	172	ASN	CA-CB	7.28	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	ASN	CA-CB	7.26	1.63	1.53
1	B	178	ALA	CA-CB	7.26	1.65	1.53
1	A	192	SER	N-CA	7.26	1.55	1.46
1	A	113	PHE	N-CA	7.25	1.55	1.46
1	B	149	PHE	N-CA	7.25	1.53	1.46
1	D	28	HIS	N-CA	7.25	1.55	1.46
1	A	80	TRP	N-CA	7.23	1.55	1.46
1	C	20	ILE	N-CA	7.23	1.54	1.46
1	A	125	TRP	CA-CB	7.20	1.66	1.53
1	B	30	SER	CA-C	-7.18	1.42	1.52
1	D	38	LYS	N-CA	7.18	1.55	1.46
1	A	52	ALA	CA-CB	7.17	1.65	1.53
1	D	117	ALA	N-CA	7.17	1.55	1.46
1	A	83	LEU	N-CA	7.16	1.54	1.45
1	C	49	GLU	N-CA	7.14	1.55	1.46
1	B	151	LEU	N-CA	7.13	1.55	1.45
1	A	47	LEU	N-CA	7.13	1.55	1.46
1	C	52	ALA	N-CA	7.13	1.54	1.46
1	C	132	THR	N-CA	7.12	1.55	1.46
1	A	188	ALA	N-CA	7.12	1.55	1.46
1	A	46	LYS	N-CA	7.11	1.55	1.46
1	C	137	LEU	N-CA	7.09	1.54	1.46
1	D	123	SER	N-CA	7.08	1.54	1.45
1	C	153	ILE	N-CA	7.08	1.54	1.46
1	D	75	ASN	N-CA	7.07	1.55	1.46
1	C	109	PHE	CA-C	7.06	1.61	1.52
1	A	77	THR	CA-CB	7.05	1.64	1.53
1	A	40	ALA	N-CA	7.04	1.55	1.46
1	D	37	VAL	N-CA	7.03	1.55	1.46
1	B	184	VAL	N-CA	7.03	1.53	1.46
1	A	17	GLU	CA-CB	-7.03	1.43	1.53
1	D	154	VAL	N-CA	7.03	1.52	1.46
1	A	33	HIS	N-CA	6.99	1.54	1.46
1	A	43	ALA	N-CA	6.99	1.54	1.46
1	B	187	TRP	N-CA	6.98	1.55	1.46
1	D	98	ALA	N-CA	6.98	1.54	1.46
1	D	184	VAL	N-CA	6.97	1.55	1.46
1	D	166	PHE	N-CA	6.96	1.53	1.46
1	B	175	VAL	CA-CB	6.96	1.63	1.54
1	A	128	LEU	N-CA	6.95	1.54	1.46
1	D	24	ILE	N-CA	6.94	1.54	1.46
1	D	120	VAL	N-CA	6.90	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	PHE	N-CA	6.90	1.55	1.46
1	D	136	LYS	N-CA	6.87	1.54	1.45
1	A	158	LEU	N-CA	6.87	1.54	1.45
1	B	138	LEU	N-CA	6.86	1.54	1.45
1	D	100	ALA	N-CA	6.85	1.55	1.46
1	C	161	MET	N-CA	6.83	1.54	1.46
1	D	40	ALA	N-CA	6.82	1.54	1.46
1	D	167	TYR	CA-CB	6.82	1.64	1.53
1	C	130	TRP	N-CA	6.78	1.54	1.46
1	D	86	ASN	CA-CB	6.76	1.63	1.53
1	A	159	LEU	N-CA	6.76	1.54	1.46
1	A	92	THR	CA-C	6.74	1.60	1.52
1	B	65	ASN	N-CA	6.73	1.54	1.46
1	A	143	TYR	CA-CB	-6.73	1.43	1.53
1	A	178	ALA	CA-CB	6.72	1.65	1.53
1	B	26	GLU	N-CA	6.67	1.54	1.46
1	B	125	TRP	N-CA	6.67	1.55	1.46
1	A	114	HIS	CA-CB	6.64	1.65	1.53
1	A	44	VAL	CA-CB	6.63	1.63	1.54
1	A	107	ASP	CA-CB	-6.62	1.42	1.53
1	B	105	SER	N-CA	6.61	1.53	1.46
1	B	186	ASN	CA-CB	6.59	1.61	1.52
1	D	196	ALA	CA-CB	6.59	1.64	1.53
1	B	78	ILE	CA-CB	6.58	1.63	1.54
1	B	198	THR	N-CA	6.55	1.54	1.46
1	B	67	ALA	CA-C	-6.54	1.44	1.52
1	C	64	LYS	N-CA	6.53	1.54	1.46
1	B	139	ILE	CA-CB	6.52	1.64	1.54
1	A	12	ASP	CA-CB	6.51	1.63	1.53
1	C	178	ALA	CA-CB	6.51	1.63	1.53
1	A	76	HIS	N-CA	6.50	1.54	1.46
1	C	126	ALA	CA-CB	-6.49	1.42	1.53
1	C	180	ALA	CA-CB	6.48	1.64	1.53
1	D	34	ALA	N-CA	6.46	1.54	1.46
1	A	50	ALA	N-CA	6.46	1.54	1.46
1	A	165	ALA	N-CA	6.46	1.54	1.46
1	A	101	ASP	N-CA	6.45	1.54	1.46
1	A	169	GLN	N-CA	6.45	1.54	1.46
1	C	60	LEU	N-CA	6.39	1.54	1.46
1	D	142	VAL	N-CA	6.38	1.54	1.46
1	B	185	VAL	CA-CB	6.37	1.61	1.54
1	D	111	ALA	CA-CB	6.37	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	VAL	CA-CB	6.36	1.61	1.54
1	B	186	ASN	N-CA	6.36	1.54	1.46
1	C	68	PHE	N-CA	6.36	1.53	1.46
1	B	45	ALA	N-CA	6.35	1.54	1.46
1	C	140	PHE	CA-CB	6.35	1.66	1.53
1	D	40	ALA	CA-CB	6.32	1.63	1.53
1	A	64	LYS	N-CA	6.30	1.54	1.46
1	A	56	HIS	CA-CB	6.29	1.61	1.53
1	A	144	ASP	CA-CB	-6.28	1.43	1.53
1	D	31	LYS	CA-CB	6.27	1.61	1.53
1	D	168	LEU	N-CA	6.27	1.54	1.46
1	C	136	LYS	N-CA	6.26	1.53	1.45
1	D	117	ALA	CA-C	-6.26	1.44	1.52
1	A	136	LYS	CA-CB	6.25	1.65	1.53
1	C	98	ALA	N-CA	6.25	1.53	1.46
1	A	117	ALA	N-CA	6.25	1.54	1.46
1	B	184	VAL	CA-CB	6.25	1.61	1.54
1	A	48	GLU	N-CA	6.24	1.53	1.46
1	D	10	ASP	CA-CB	6.23	1.61	1.53
1	C	21	SER	CA-CB	6.23	1.63	1.53
1	C	53	LYS	N-CA	6.22	1.54	1.46
1	C	67	ALA	N-CA	6.22	1.54	1.46
1	D	71	ALA	N-CA	6.22	1.54	1.46
1	C	11	TRP	N-CA	6.21	1.53	1.46
1	C	23	GLN	N-CA	6.20	1.53	1.46
1	A	192	SER	CA-CB	6.19	1.63	1.53
1	D	162	TRP	CA-CB	-6.19	1.42	1.53
1	A	67	ALA	N-CA	6.19	1.54	1.46
1	C	56	HIS	CA-CB	6.18	1.61	1.53
1	B	62	ASN	CA-C	-6.15	1.44	1.52
1	C	95	LEU	N-CA	6.14	1.53	1.46
1	C	171	LYS	CA-C	-6.14	1.44	1.52
1	A	30	SER	CA-C	-6.13	1.44	1.52
1	A	196	ALA	N-CA	6.12	1.54	1.46
1	C	8	ASP	N-CA	6.10	1.53	1.45
1	A	137	LEU	CA-CB	6.08	1.62	1.53
1	A	101	ASP	CA-CB	6.07	1.63	1.53
1	D	100	ALA	CA-CB	6.07	1.63	1.53
1	A	176	ASP	N-CA	6.06	1.53	1.46
1	C	109	PHE	CA-CB	6.05	1.62	1.53
1	C	188	ALA	N-CA	6.05	1.53	1.46
1	D	119	THR	N-CA	6.05	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	48	GLU	N-CA	6.04	1.53	1.46
1	B	193	ARG	N-CA	6.03	1.54	1.46
1	D	80	TRP	N-CA	6.03	1.53	1.46
1	C	147	THR	N-CA	6.01	1.53	1.45
1	D	116	ALA	N-CA	6.01	1.54	1.46
1	C	153	ILE	CA-CB	-6.00	1.47	1.54
1	D	118	THR	N-CA	6.00	1.53	1.46
1	B	61	LEU	N-CA	5.99	1.53	1.46
1	A	4	TYR	CA-CB	5.99	1.62	1.53
1	A	24	ILE	N-CA	5.98	1.53	1.46
1	A	139	ILE	CA-CB	5.98	1.63	1.54
1	D	73	HIS	CA-CB	5.98	1.62	1.53
1	D	118	THR	CA-CB	5.96	1.61	1.53
1	A	153	ILE	N-CA	5.95	1.53	1.46
1	A	100	ALA	N-CA	5.95	1.54	1.46
1	A	20	ILE	N-CA	5.93	1.53	1.46
1	A	82	ASN	N-CA	5.93	1.54	1.46
1	A	123	SER	N-CA	5.92	1.53	1.45
1	A	55	ASP	N-CA	5.90	1.54	1.46
1	D	19	HIS	N-CA	5.90	1.53	1.46
1	A	92	THR	N-CA	5.90	1.53	1.45
1	B	69	ASN	N-CA	5.89	1.53	1.46
1	B	53	LYS	N-CA	5.88	1.53	1.46
1	D	50	ALA	N-CA	5.87	1.53	1.46
1	B	131	ASP	N-CA	5.86	1.53	1.46
1	C	13	TYR	N-CA	5.85	1.53	1.46
1	A	112	GLN	N-CA	5.84	1.53	1.46
1	B	130	TRP	CA-C	-5.84	1.45	1.52
1	A	105	SER	CA-CB	5.83	1.63	1.53
1	A	184	VAL	CA-CB	-5.83	1.48	1.54
1	C	64	LYS	CA-C	-5.83	1.44	1.52
1	A	194	TYR	N-CA	5.82	1.53	1.46
1	B	97	ALA	N-CA	5.82	1.53	1.46
1	D	99	ILE	CA-CB	-5.80	1.46	1.54
1	D	169	GLN	CA-C	-5.79	1.45	1.52
1	B	77	THR	N-CA	5.79	1.53	1.46
1	D	60	LEU	CA-CB	5.78	1.62	1.53
1	C	96	ALA	N-CA	5.78	1.53	1.46
1	B	6	LEU	CA-C	-5.76	1.46	1.52
1	D	69	ASN	CA-CB	5.75	1.62	1.53
1	A	15	ALA	CA-CB	5.74	1.64	1.53
1	D	10	ASP	N-CA	5.73	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	HIS	N-CA	5.73	1.53	1.46
1	D	121	GLN	CA-CB	5.72	1.61	1.53
1	D	181	PHE	CA-CB	5.72	1.62	1.53
1	B	97	ALA	CA-CB	5.71	1.63	1.53
1	C	7	PRO	CA-CB	5.70	1.60	1.53
1	B	130	TRP	N-CA	5.68	1.52	1.46
1	C	190	VAL	N-CA	5.66	1.53	1.46
1	D	176	ASP	N-CA	5.65	1.53	1.46
1	C	44	VAL	N-CA	5.64	1.53	1.46
1	B	158	LEU	CA-C	5.64	1.59	1.52
1	C	196	ALA	CA-CB	5.64	1.62	1.53
1	C	61	LEU	N-CA	5.63	1.53	1.46
1	D	103	PHE	CA-CB	5.63	1.62	1.53
1	D	120	VAL	CA-CB	5.62	1.60	1.54
1	C	133	LEU	N-CA	5.62	1.53	1.46
1	A	34	ALA	N-CA	5.61	1.53	1.46
1	A	168	LEU	CA-CB	5.59	1.62	1.53
1	A	98	ALA	N-CA	5.59	1.52	1.46
1	B	25	ASN	N-CA	5.59	1.53	1.46
1	C	189	ASP	N-CA	5.59	1.53	1.46
1	D	26	GLU	CA-CB	5.58	1.62	1.53
1	D	197	ALA	N-CA	5.58	1.53	1.46
1	B	183	ASN	N-CA	5.53	1.53	1.46
1	B	77	THR	CA-CB	5.53	1.62	1.53
1	D	168	LEU	CA-CB	5.51	1.63	1.53
1	C	32	HIS	CA-C	-5.51	1.45	1.52
1	D	52	ALA	N-CA	5.51	1.53	1.46
1	C	29	HIS	CA-CB	5.50	1.62	1.53
1	D	167	TYR	CA-C	-5.50	1.45	1.52
1	B	131	ASP	CA-CB	5.49	1.61	1.53
1	B	34	ALA	CA-C	-5.47	1.45	1.52
1	B	23	GLN	CA-CB	5.47	1.62	1.53
1	C	36	TYR	N-CA	5.47	1.52	1.46
1	A	41	ASN	CA-CB	-5.46	1.44	1.53
1	A	183	ASN	N-CA	5.45	1.53	1.46
1	A	121	GLN	N-CA	5.45	1.54	1.46
1	A	51	ARG	N-CA	5.44	1.53	1.46
1	B	113	PHE	CA-CB	5.41	1.62	1.53
1	D	65	ASN	CA-CB	5.41	1.62	1.53
1	C	186	ASN	CA-CB	5.41	1.60	1.52
1	C	108	LYS	N-CA	5.40	1.53	1.46
1	D	179	LYS	N-CA	5.40	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	LYS	N-CA	5.38	1.53	1.46
1	B	159	LEU	N-CA	5.37	1.52	1.46
1	C	68	PHE	CA-C	-5.37	1.46	1.52
1	D	192	SER	CA-CB	5.35	1.62	1.53
1	D	49	GLU	N-CA	5.35	1.52	1.46
1	B	178	ALA	N-CA	5.34	1.53	1.46
1	A	6	LEU	CA-CB	5.31	1.64	1.53
1	C	146	GLN	N-CA	5.30	1.54	1.46
1	B	194	TYR	N-CA	5.29	1.52	1.46
1	D	125	TRP	N-CA	5.29	1.52	1.45
1	A	91	PRO	N-CA	5.28	1.52	1.47
1	B	188	ALA	N-CA	5.27	1.53	1.46
1	C	92	THR	CA-CB	5.27	1.66	1.53
1	A	90	LYS	CA-C	-5.26	1.46	1.52
1	B	66	LEU	CA-CB	5.26	1.61	1.53
1	D	89	ASP	CA-CB	5.26	1.62	1.53
1	C	44	VAL	CA-CB	-5.25	1.48	1.54
1	A	44	VAL	N-CA	5.25	1.53	1.46
1	B	52	ALA	CA-CB	5.25	1.61	1.53
1	A	147	THR	N-CA	5.24	1.52	1.45
1	C	79	TRP	N-CA	5.24	1.52	1.46
1	C	184	VAL	CA-CB	-5.22	1.47	1.54
1	B	67	ALA	CA-CB	5.21	1.61	1.53
1	C	113	PHE	N-CA	5.21	1.52	1.46
1	C	61	LEU	CA-C	-5.19	1.46	1.52
1	D	12	ASP	N-CA	5.19	1.52	1.45
1	C	6	LEU	CA-C	-5.17	1.47	1.52
1	D	82	ASN	CA-C	5.17	1.59	1.52
1	A	121	GLN	CA-C	-5.15	1.47	1.53
1	C	196	ALA	N-CA	5.15	1.52	1.46
1	D	139	ILE	CA-CB	5.14	1.61	1.54
1	A	78	ILE	N-CA	5.12	1.53	1.46
1	C	170	TYR	CA-CB	5.10	1.61	1.53
1	D	128	LEU	N-CA	5.09	1.52	1.46
1	C	60	LEU	CA-C	-5.08	1.45	1.52
1	C	17	GLU	N-CA	5.08	1.53	1.45
1	D	7	PRO	CA-CB	5.08	1.60	1.53
1	B	146	GLN	CA-CB	5.06	1.59	1.53
1	B	155	PRO	CA-CB	5.04	1.60	1.53
1	C	151	LEU	N-CA	5.04	1.52	1.45
1	C	185	VAL	N-CA	5.01	1.52	1.46
1	D	196	ALA	N-CA	5.00	1.52	1.46

All (847) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	SER	O-C-N	13.97	132.73	121.83
1	D	30	SER	N-CA-C	13.88	126.49	111.36
1	C	153	ILE	CA-CB-CG2	12.64	131.99	110.50
1	C	153	ILE	CA-C-N	-12.51	111.53	123.04
1	C	153	ILE	C-N-CA	-12.51	111.53	123.04
1	C	109	PHE	N-CA-C	-12.37	97.30	111.03
1	B	40	ALA	N-CA-CB	-12.27	92.28	110.07
1	B	179	LYS	N-CA-C	-12.21	98.87	113.88
1	C	54	GLU	CA-C-N	-11.98	106.11	123.00
1	C	54	GLU	C-N-CA	-11.98	106.11	123.00
1	B	44	VAL	N-CA-CB	-11.85	94.42	110.54
1	A	146	GLN	N-CA-C	11.59	127.47	112.41
1	D	69	ASN	CA-CB-CG	-11.40	101.20	112.60
1	A	153	ILE	CA-C-N	-11.27	114.48	122.59
1	A	153	ILE	C-N-CA	-11.27	114.48	122.59
1	B	47	LEU	N-CA-C	-11.27	97.66	111.40
1	C	150	PRO	CB-CA-C	-10.81	94.42	110.20
1	A	97	ALA	N-CA-C	-10.80	99.84	113.23
1	A	109	PHE	N-CA-CB	-10.80	94.35	110.01
1	D	145	GLU	CA-CB-CG	10.74	135.57	114.10
1	A	105	SER	N-CA-CB	-10.54	95.22	111.56
1	B	149	PHE	N-CA-C	-10.42	98.75	108.13
1	A	126	ALA	N-CA-C	-10.41	93.07	109.72
1	B	169	GLN	N-CA-CB	-10.20	97.02	110.59
1	D	15	ALA	N-CA-C	10.19	124.81	112.38
1	C	20	ILE	N-CA-C	-10.11	93.49	108.45
1	C	101	ASP	CA-CB-CG	-10.10	102.50	112.60
1	A	107	ASP	CA-CB-CG	9.79	122.39	112.60
1	D	121	GLN	N-CA-CB	-9.73	94.02	110.46
1	D	102	ALA	N-CA-C	9.71	121.95	111.36
1	C	186	ASN	N-CA-CB	-9.65	94.50	110.53
1	D	161	MET	N-CA-CB	9.64	125.19	110.44
1	A	154	VAL	CA-C-O	9.61	124.82	119.15
1	D	84	SER	CA-C-N	9.60	129.31	118.85
1	D	84	SER	C-N-CA	9.60	129.31	118.85
1	D	111	ALA	N-CA-C	-9.59	100.34	112.90
1	B	158	LEU	N-CA-CB	-9.54	94.01	111.37
1	B	6	LEU	CA-C-O	9.50	126.78	119.46
1	A	101	ASP	CA-CB-CG	-9.49	103.11	112.60
1	B	86	ASN	CA-CB-CG	-9.49	103.11	112.60
1	D	120	VAL	CA-C-N	-9.49	109.09	123.14
1	D	120	VAL	C-N-CA	-9.49	109.09	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	VAL	N-CA-CB	-9.49	99.61	111.94
1	D	117	ALA	N-CA-CB	-9.48	95.66	110.44
1	B	146	GLN	N-CA-C	9.46	126.38	111.81
1	C	82	ASN	CA-C-N	-9.40	107.83	122.59
1	C	82	ASN	C-N-CA	-9.40	107.83	122.59
1	B	46	LYS	N-CA-CB	-9.40	95.70	110.46
1	A	149	PHE	N-CA-C	-9.37	99.73	108.07
1	B	67	ALA	N-CA-CB	-9.36	95.78	110.28
1	A	12	ASP	N-CA-CB	-9.32	96.02	110.56
1	D	140	PHE	CA-C-N	-9.26	110.09	123.05
1	D	140	PHE	C-N-CA	-9.26	110.09	123.05
1	B	27	LEU	N-CA-C	-9.21	100.83	112.90
1	B	168	LEU	CA-C-N	-9.21	106.52	122.36
1	B	168	LEU	C-N-CA	-9.21	106.52	122.36
1	C	185	VAL	CB-CA-C	-9.20	97.62	111.33
1	C	140	PHE	CA-CB-CG	-9.18	104.62	113.80
1	C	172	ASN	N-CA-CB	-9.18	97.26	110.57
1	B	146	GLN	CB-CG-CD	9.16	128.18	112.60
1	A	92	THR	N-CA-CB	-9.10	96.46	111.66
1	C	109	PHE	O-C-N	9.09	131.85	122.03
1	C	149	PHE	CB-CA-C	9.06	122.78	110.37
1	B	9	LEU	N-CA-C	-8.99	97.55	110.59
1	A	114	HIS	N-CA-CB	-8.97	95.51	110.39
1	B	11	TRP	CA-C-N	-8.94	106.79	122.07
1	B	11	TRP	C-N-CA	-8.94	106.79	122.07
1	C	179	LYS	N-CA-CB	-8.93	96.54	110.30
1	A	119	THR	CB-CA-C	-8.93	96.65	111.02
1	D	141	GLN	N-CA-C	-8.93	93.97	108.52
1	A	74	VAL	CB-CA-C	-8.85	97.92	112.26
1	A	138	LEU	N-CA-CB	-8.83	97.88	111.56
1	D	89	ASP	CA-CB-CG	-8.81	103.79	112.60
1	D	73	HIS	N-CA-CB	-8.77	97.18	110.16
1	C	85	PRO	CB-CA-C	-8.74	97.43	112.64
1	D	146	GLN	CB-CG-CD	8.74	127.45	112.60
1	B	190	VAL	CA-CB-CG1	8.73	125.24	110.40
1	D	117	ALA	CA-C-N	-8.72	108.80	122.67
1	D	117	ALA	C-N-CA	-8.72	108.80	122.67
1	C	37	VAL	CB-CA-C	-8.71	100.63	112.04
1	C	126	ALA	N-CA-C	-8.70	95.58	109.59
1	C	40	ALA	N-CA-CB	-8.69	97.25	110.20
1	C	30	SER	N-CA-C	8.68	120.75	111.28
1	C	55	ASP	N-CA-CB	-8.68	97.12	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	LYS	CA-C-N	-8.68	104.94	122.55
1	C	171	LYS	C-N-CA	-8.68	104.94	122.55
1	A	109	PHE	N-CA-C	-8.63	101.83	111.07
1	D	126	ALA	N-CA-CB	8.62	124.11	110.57
1	C	66	LEU	N-CA-CB	-8.60	97.38	110.20
1	A	174	LYS	CA-C-N	-8.59	106.56	120.64
1	A	174	LYS	C-N-CA	-8.59	106.56	120.64
1	A	153	ILE	N-CA-CB	-8.56	98.74	110.56
1	D	4	TYR	N-CA-C	-8.52	98.23	110.59
1	B	117	ALA	N-CA-CB	-8.47	97.14	110.28
1	C	62	ASN	N-CA-CB	-8.47	97.15	110.28
1	A	92	THR	CA-CB-CG2	-8.42	96.18	110.50
1	D	37	VAL	CA-CB-CG1	-8.42	96.08	110.40
1	B	186	ASN	CB-CA-C	-8.39	97.58	111.68
1	C	15	ALA	N-CA-C	8.37	122.46	111.75
1	C	146	GLN	N-CA-CB	-8.35	95.41	111.53
1	B	142	VAL	N-CA-CB	-8.34	95.43	110.95
1	C	109	PHE	N-CA-CB	-8.33	97.90	109.98
1	C	165	ALA	N-CA-CB	-8.33	97.70	110.44
1	A	138	LEU	N-CA-C	-8.29	96.11	108.79
1	C	176	ASP	CA-C-N	-8.24	106.49	120.58
1	C	176	ASP	C-N-CA	-8.24	106.49	120.58
1	B	10	ASP	CB-CA-C	-8.19	97.95	111.13
1	A	153	ILE	CA-CB-CG1	-8.18	96.50	110.40
1	B	143	TYR	N-CA-C	-8.14	96.49	109.59
1	B	116	ALA	CA-C-N	-8.08	108.03	120.31
1	B	116	ALA	C-N-CA	-8.08	108.03	120.31
1	C	109	PHE	CB-CA-C	-8.08	98.42	110.95
1	B	27	LEU	N-CA-CB	-8.06	98.23	110.33
1	A	125	TRP	CB-CA-C	-8.05	92.72	110.67
1	C	180	ALA	N-CA-CB	-7.99	97.12	110.39
1	A	151	LEU	N-CA-CB	-7.94	99.01	110.36
1	C	177	PHE	N-CA-C	-7.93	101.94	111.69
1	D	154	VAL	CA-C-N	7.93	129.09	120.13
1	D	154	VAL	C-N-CA	7.93	129.09	120.13
1	C	19	HIS	CA-CB-CG	-7.92	105.88	113.80
1	C	185	VAL	CA-CB-CG1	-7.92	96.94	110.40
1	C	141	GLN	CA-CB-CG	-7.90	98.29	114.10
1	B	36	TYR	N-CA-CB	-7.89	98.62	110.07
1	B	60	LEU	N-CA-CB	-7.88	98.49	110.16
1	B	49	GLU	N-CA-CB	-7.88	97.17	110.41
1	A	3	GLU	N-CA-CB	-7.87	99.60	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	THR	CB-CA-C	-7.86	93.56	110.45
1	D	169	GLN	N-CA-CB	-7.84	99.02	110.40
1	A	128	LEU	N-CA-C	-7.84	96.96	109.59
1	D	150	PRO	CB-CA-C	-7.84	98.80	110.17
1	A	52	ALA	N-CA-CB	-7.82	98.55	110.20
1	D	147	THR	N-CA-CB	-7.78	98.15	111.69
1	C	137	LEU	N-CA-C	-7.76	96.57	109.07
1	D	31	LYS	N-CA-CB	-7.76	98.44	110.39
1	D	6	LEU	CA-C-O	7.72	125.41	119.46
1	B	75	ASN	CA-C-N	-7.72	107.56	120.68
1	B	75	ASN	C-N-CA	-7.72	107.56	120.68
1	C	77	THR	N-CA-CB	-7.69	98.38	110.22
1	D	9	LEU	N-CA-C	-7.69	99.44	110.59
1	A	195	ALA	N-CA-CB	-7.67	98.38	110.28
1	A	91	PRO	N-CA-C	-7.67	99.70	111.13
1	C	69	ASN	CA-CB-CG	-7.67	104.93	112.60
1	D	131	ASP	N-CA-CB	-7.67	97.92	110.42
1	A	41	ASN	CA-CB-CG	7.66	120.26	112.60
1	D	10	ASP	CB-CA-C	-7.65	98.37	111.46
1	A	189	ASP	CA-CB-CG	-7.64	104.96	112.60
1	B	74	VAL	CA-CB-CG1	7.64	123.39	110.40
1	D	37	VAL	CB-CA-C	-7.62	99.92	112.26
1	B	154	VAL	O-C-N	7.61	127.39	121.46
1	C	176	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	37	VAL	CA-C-N	-7.56	107.83	120.68
1	B	37	VAL	C-N-CA	-7.56	107.83	120.68
1	A	185	VAL	CA-C-N	-7.55	111.97	123.14
1	A	185	VAL	C-N-CA	-7.55	111.97	123.14
1	C	185	VAL	CA-C-N	-7.54	111.61	122.77
1	C	185	VAL	C-N-CA	-7.54	111.61	122.77
1	C	157	LEU	CB-CA-C	-7.54	99.23	110.24
1	D	69	ASN	N-CA-CB	-7.51	99.04	110.16
1	B	54	GLU	CB-CA-C	-7.50	101.81	111.86
1	A	186	ASN	CA-CB-CG	-7.50	105.11	112.60
1	A	138	LEU	O-C-N	7.49	131.43	123.42
1	C	10	ASP	N-CA-C	-7.48	103.72	112.92
1	D	111	ALA	N-CA-CB	-7.48	99.11	110.33
1	B	52	ALA	CB-CA-C	-7.47	98.85	110.81
1	D	168	LEU	CA-C-N	-7.47	109.49	122.79
1	D	168	LEU	C-N-CA	-7.47	109.49	122.79
1	B	30	SER	N-CA-C	7.47	121.50	112.38
1	A	120	VAL	CA-C-N	-7.45	111.79	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	VAL	C-N-CA	-7.45	111.79	123.12
1	C	48	GLU	N-CA-C	-7.45	103.10	111.07
1	B	154	VAL	CB-CA-C	-7.44	102.22	110.78
1	C	40	ALA	N-CA-C	-7.44	102.54	111.69
1	C	154	VAL	N-CA-C	-7.43	99.28	108.05
1	D	118	THR	CA-CB-OG1	-7.41	98.49	109.60
1	C	150	PRO	N-CA-CB	-7.41	94.13	102.72
1	D	27	LEU	N-CA-C	-7.40	103.29	111.36
1	C	177	PHE	N-CA-CB	-7.39	99.18	110.20
1	D	103	PHE	CA-CB-CG	-7.39	106.41	113.80
1	D	99	ILE	CB-CG1-CD1	-7.39	98.29	113.80
1	A	86	ASN	CA-CB-CG	-7.35	105.25	112.60
1	C	114	HIS	N-CA-CB	-7.34	99.26	110.20
1	D	142	VAL	N-CA-CB	-7.32	100.46	110.56
1	B	69	ASN	CA-C-N	-7.31	109.76	120.28
1	B	69	ASN	C-N-CA	-7.31	109.76	120.28
1	B	43	ALA	N-CA-C	-7.31	102.70	111.69
1	C	149	PHE	N-CA-CB	-7.26	102.13	111.35
1	A	101	ASP	N-CA-CB	-7.22	99.17	110.44
1	D	98	ALA	N-CA-C	-7.22	103.34	111.07
1	C	73	HIS	N-CA-CB	-7.22	99.09	110.28
1	B	126	ALA	N-CA-C	-7.21	97.97	109.59
1	D	23	GLN	N-CA-C	-7.21	103.35	111.14
1	A	184	VAL	CB-CA-C	7.21	119.85	110.84
1	A	114	HIS	CA-CB-CG	-7.20	106.60	113.80
1	C	138	LEU	N-CA-CB	-7.20	99.96	111.62
1	C	69	ASN	N-CA-CB	-7.19	99.49	110.20
1	D	168	LEU	N-CA-CB	-7.19	98.10	110.32
1	B	178	ALA	N-CA-CB	-7.15	98.40	110.49
1	B	35	THR	N-CA-CB	-7.14	99.61	110.33
1	C	185	VAL	N-CA-CB	-7.14	101.53	110.31
1	C	24	ILE	CA-CB-CG2	-7.13	98.37	110.50
1	D	65	ASN	N-CA-CB	-7.12	99.33	110.30
1	B	67	ALA	CA-C-N	-7.12	110.76	120.44
1	B	67	ALA	C-N-CA	-7.12	110.76	120.44
1	B	162	TRP	N-CA-C	-7.12	100.94	110.55
1	D	126	ALA	N-CA-C	-7.10	97.64	109.07
1	C	179	LYS	CB-CA-C	-7.09	95.91	110.38
1	A	141	GLN	N-CA-C	-7.08	95.62	108.02
1	A	82	ASN	CB-CA-C	-7.08	97.26	110.36
1	A	186	ASN	N-CA-CB	-7.08	98.50	110.46
1	C	145	GLU	N-CA-C	-7.07	104.14	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASN	CA-CB-CG	-7.06	105.54	112.60
1	D	196	ALA	N-CA-C	-7.03	103.37	112.23
1	C	92	THR	CB-CA-C	-7.02	95.50	109.33
1	B	62	ASN	CA-C-N	-7.02	110.32	120.29
1	B	62	ASN	C-N-CA	-7.02	110.32	120.29
1	A	44	VAL	N-CA-CB	-7.02	98.07	110.77
1	C	194	TYR	N-CA-CB	-7.01	99.50	110.30
1	B	131	ASP	N-CA-CB	-7.01	98.60	110.16
1	A	53	LYS	CB-CA-C	-7.00	97.41	110.36
1	A	113	PHE	CA-C-N	-6.99	109.04	120.72
1	A	113	PHE	C-N-CA	-6.99	109.04	120.72
1	C	95	LEU	N-CA-CB	-6.99	99.84	110.12
1	B	72	GLY	CA-C-N	-6.98	110.95	120.44
1	B	72	GLY	C-N-CA	-6.98	110.95	120.44
1	C	120	VAL	CB-CA-C	-6.98	101.43	111.34
1	B	99	ILE	N-CA-CB	-6.97	103.30	110.62
1	C	141	GLN	CB-CA-C	-6.97	99.42	110.79
1	C	142	VAL	CA-CB-CG2	-6.97	98.56	110.40
1	A	124	GLY	CA-C-O	-6.96	115.02	121.63
1	C	118	THR	CA-CB-CG2	-6.96	98.67	110.50
1	B	136	LYS	CA-C-N	6.95	131.88	122.84
1	B	136	LYS	C-N-CA	6.95	131.88	122.84
1	D	32	HIS	CA-C-N	-6.94	110.28	120.28
1	D	32	HIS	C-N-CA	-6.94	110.28	120.28
1	A	148	ASN	N-CA-C	6.94	125.58	110.80
1	D	7	PRO	CA-C-N	-6.92	110.69	122.67
1	D	7	PRO	C-N-CA	-6.92	110.69	122.67
1	C	139	ILE	CA-C-N	-6.92	111.19	122.81
1	C	139	ILE	C-N-CA	-6.92	111.19	122.81
1	A	100	ALA	CA-C-N	-6.91	109.50	121.66
1	A	100	ALA	C-N-CA	-6.91	109.50	121.66
1	D	141	GLN	N-CA-CB	-6.90	99.71	110.55
1	B	44	VAL	CA-CB-CG2	-6.89	98.68	110.40
1	B	4	TYR	N-CA-C	-6.89	100.79	110.50
1	D	12	ASP	CA-CB-CG	-6.89	105.71	112.60
1	B	146	GLN	N-CA-CB	-6.88	101.20	111.25
1	A	138	LEU	CA-C-O	-6.84	113.91	121.23
1	B	97	ALA	N-CA-C	-6.84	104.75	113.23
1	A	111	ALA	N-CA-C	-6.83	103.28	111.69
1	B	173	VAL	CA-CB-CG1	6.83	122.02	110.40
1	D	146	GLN	N-CA-CB	-6.82	100.75	111.39
1	A	146	GLN	N-CA-CB	-6.81	99.96	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	HIS	CA-C-N	-6.81	110.05	122.38
1	C	164	HIS	C-N-CA	-6.81	110.05	122.38
1	D	73	HIS	CA-CB-CG	-6.81	106.99	113.80
1	B	142	VAL	CB-CA-C	-6.80	101.54	111.68
1	C	137	LEU	CA-C-N	-6.80	111.48	122.36
1	C	137	LEU	C-N-CA	-6.80	111.48	122.36
1	D	72	GLY	CA-C-N	-6.79	110.64	120.29
1	D	72	GLY	C-N-CA	-6.79	110.64	120.29
1	D	82	ASN	CA-C-N	-6.79	112.15	122.81
1	D	82	ASN	C-N-CA	-6.79	112.15	122.81
1	B	154	VAL	N-CA-CB	-6.78	102.89	111.23
1	A	153	ILE	CB-CA-C	-6.78	101.92	111.21
1	C	35	THR	N-CA-CB	-6.76	100.15	110.16
1	D	154	VAL	O-C-N	6.75	126.72	121.46
1	B	147	THR	N-CA-CB	-6.74	98.98	111.52
1	C	120	VAL	CA-CB-CG1	-6.74	98.94	110.40
1	D	83	LEU	CD1-CG-CD2	-6.74	95.97	110.80
1	C	125	TRP	CB-CA-C	-6.74	95.65	110.67
1	C	152	GLY	N-CA-C	6.72	124.30	115.36
1	A	30	SER	N-CA-C	6.71	121.07	113.01
1	B	20	ILE	N-CA-C	-6.70	95.41	109.34
1	A	136	LYS	CB-CA-C	-6.68	95.70	109.94
1	D	177	PHE	N-CA-C	-6.68	103.47	111.69
1	A	43	ALA	N-CA-CB	-6.68	100.27	110.16
1	B	42	ASP	N-CA-CB	-6.68	99.52	110.40
1	A	196	ALA	N-CA-CB	-6.68	100.25	110.20
1	A	69	ASN	CA-C-N	-6.67	110.17	120.31
1	A	69	ASN	C-N-CA	-6.67	110.17	120.31
1	C	24	ILE	N-CA-CB	6.67	118.35	110.55
1	D	5	THR	CB-CA-C	-6.66	98.24	110.62
1	C	196	ALA	N-CA-CB	-6.65	99.97	110.28
1	D	82	ASN	CA-CB-CG	6.65	119.25	112.60
1	A	161	MET	N-CA-CB	6.65	120.27	110.56
1	C	175	VAL	N-CA-C	6.65	120.34	111.17
1	B	124	GLY	CA-C-N	-6.64	111.83	122.53
1	B	124	GLY	C-N-CA	-6.64	111.83	122.53
1	D	158	LEU	CD1-CG-CD2	-6.64	96.19	110.80
1	B	109	PHE	N-CA-C	-6.64	104.13	111.36
1	D	3	GLU	N-CA-CB	-6.63	100.36	110.45
1	C	140	PHE	N-CA-CB	-6.63	100.46	111.20
1	A	40	ALA	CB-CA-C	-6.62	99.60	110.85
1	A	63	GLU	N-CA-CB	-6.61	99.63	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	SER	N-CA-CB	-6.61	100.99	110.44
1	C	52	ALA	N-CA-CB	-6.60	100.44	110.01
1	C	9	LEU	N-CA-C	-6.60	100.69	110.46
1	D	74	VAL	CA-CB-CG1	-6.60	99.18	110.40
1	B	23	GLN	N-CA-CB	-6.59	100.14	110.30
1	D	147	THR	CA-CB-CG2	6.59	121.70	110.50
1	B	46	LYS	CA-C-N	-6.58	109.73	120.71
1	B	46	LYS	C-N-CA	-6.58	109.73	120.71
1	C	64	LYS	N-CA-CB	-6.58	100.17	110.30
1	B	125	TRP	CB-CA-C	-6.57	95.88	111.65
1	B	10	ASP	N-CA-C	-6.56	103.60	112.26
1	C	193	ARG	CA-C-N	-6.56	109.53	120.68
1	C	193	ARG	C-N-CA	-6.56	109.53	120.68
1	B	63	GLU	N-CA-C	-6.55	104.22	111.36
1	A	130	TRP	N-CA-CB	-6.55	99.68	110.68
1	D	30	SER	CA-CB-OG	-6.55	98.00	111.10
1	A	15	ALA	N-CA-CB	-6.55	98.40	110.32
1	A	90	LYS	CA-C-N	-6.55	114.04	120.52
1	A	90	LYS	C-N-CA	-6.55	114.04	120.52
1	B	19	HIS	CA-C-N	-6.55	110.19	121.97
1	B	19	HIS	C-N-CA	-6.55	110.19	121.97
1	B	26	GLU	CA-C-N	-6.54	109.48	121.52
1	B	26	GLU	C-N-CA	-6.54	109.48	121.52
1	B	114	HIS	CA-C-N	-6.54	111.54	120.44
1	B	114	HIS	C-N-CA	-6.54	111.54	120.44
1	A	8	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	84	SER	CA-C-N	6.54	126.77	119.32
1	C	84	SER	C-N-CA	6.54	126.77	119.32
1	C	101	ASP	CB-CA-C	-6.53	99.82	110.79
1	B	20	ILE	CA-C-N	6.53	129.98	120.71
1	B	20	ILE	C-N-CA	6.53	129.98	120.71
1	C	70	LEU	N-CA-C	-6.53	104.25	111.36
1	C	148	ASN	CA-CB-CG	-6.52	106.08	112.60
1	B	50	ALA	N-CA-C	-6.52	104.02	112.23
1	D	57	SER	CA-C-N	-6.52	112.80	122.83
1	D	57	SER	C-N-CA	-6.52	112.80	122.83
1	C	156	LEU	CA-C-N	-6.51	111.57	121.86
1	C	156	LEU	C-N-CA	-6.51	111.57	121.86
1	D	37	VAL	CA-CB-CG2	-6.51	99.33	110.40
1	D	107	ASP	CA-CB-CG	-6.50	106.10	112.60
1	A	100	ALA	CA-C-O	6.50	127.37	119.31
1	D	10	ASP	N-CA-C	-6.50	102.01	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	MET	CG-SD-CE	6.49	115.17	100.90
1	D	85	PRO	CB-CA-C	-6.48	102.84	112.55
1	B	86	ASN	CB-CA-C	-6.47	99.62	110.56
1	A	143	TYR	CA-CB-CG	6.47	125.55	113.90
1	C	34	ALA	CA-C-N	-6.47	111.10	120.29
1	C	34	ALA	C-N-CA	-6.47	111.10	120.29
1	A	96	ALA	CA-C-N	-6.46	110.28	121.66
1	A	96	ALA	C-N-CA	-6.46	110.28	121.66
1	D	37	VAL	CA-C-N	-6.46	111.12	120.29
1	D	37	VAL	C-N-CA	-6.46	111.12	120.29
1	B	130	TRP	CA-C-N	-6.44	113.11	122.19
1	B	130	TRP	C-N-CA	-6.44	113.11	122.19
1	D	191	GLN	CA-C-O	6.44	127.38	120.55
1	D	181	PHE	CB-CA-C	-6.43	99.75	110.68
1	B	33	HIS	N-CA-C	6.42	118.28	111.28
1	B	77	THR	CA-C-N	-6.41	112.28	121.52
1	B	77	THR	C-N-CA	-6.41	112.28	121.52
1	B	98	ALA	N-CA-C	-6.41	103.91	111.03
1	D	4	TYR	N-CA-CB	-6.41	100.68	110.42
1	B	98	ALA	CB-CA-C	6.40	120.87	110.95
1	C	103	PHE	N-CA-C	6.40	120.40	112.59
1	D	131	ASP	CA-CB-CG	-6.40	106.20	112.60
1	C	151	LEU	N-CA-CB	-6.39	100.97	110.17
1	A	167	TYR	N-CA-C	6.39	119.06	111.33
1	A	113	PHE	N-CA-CB	-6.38	100.48	110.06
1	D	29	HIS	N-CA-C	-6.38	104.25	111.14
1	D	60	LEU	N-CA-C	6.38	119.04	111.71
1	C	42	ASP	CB-CA-C	-6.38	98.06	110.11
1	D	45	ALA	CA-C-N	-6.36	110.64	120.31
1	D	45	ALA	C-N-CA	-6.36	110.64	120.31
1	D	99	ILE	CA-CB-CG2	6.36	121.31	110.50
1	D	100	ALA	N-CA-CB	-6.36	100.04	110.40
1	D	135	ASN	CA-C-N	-6.34	111.94	122.21
1	D	135	ASN	C-N-CA	-6.34	111.94	122.21
1	C	167	TYR	N-CA-CB	6.33	120.48	109.72
1	D	79	TRP	N-CA-CB	-6.33	100.47	110.28
1	A	147	THR	OG1-CB-CG2	6.33	121.95	109.30
1	B	129	GLY	CA-C-N	-6.33	114.27	123.00
1	B	129	GLY	C-N-CA	-6.33	114.27	123.00
1	A	69	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	146	GLN	CB-CG-CD	6.32	123.33	112.60
1	B	34	ALA	CA-C-N	-6.32	109.90	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	ALA	C-N-CA	-6.32	109.90	121.52
1	C	107	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	116	ALA	N-CA-CB	-6.31	100.50	110.22
1	B	77	THR	N-CA-CB	-6.31	100.51	110.22
1	A	173	VAL	N-CA-C	6.30	122.45	109.34
1	B	151	LEU	N-CA-CB	-6.30	101.34	110.36
1	C	48	GLU	N-CA-CB	-6.30	100.87	110.01
1	B	79	TRP	CA-CB-CG	6.29	125.56	113.60
1	B	125	TRP	CB-CG-CD2	-6.29	117.99	126.80
1	A	188	ALA	N-CA-C	-6.28	104.53	111.82
1	A	26	GLU	N-CA-CB	-6.28	100.84	110.20
1	D	153	ILE	CA-CB-CG2	-6.28	99.83	110.50
1	B	57	SER	N-CA-CB	6.27	119.88	110.22
1	B	78	ILE	N-CA-CB	-6.27	97.77	111.81
1	B	97	ALA	N-CA-CB	-6.25	100.68	110.44
1	B	35	THR	CA-CB-OG1	-6.25	100.22	109.60
1	C	125	TRP	CA-C-N	-6.25	113.87	122.93
1	C	125	TRP	C-N-CA	-6.25	113.87	122.93
1	B	71	ALA	N-CA-CB	-6.24	100.92	110.16
1	C	126	ALA	CA-C-N	-6.23	111.65	122.37
1	C	126	ALA	C-N-CA	-6.23	111.65	122.37
1	B	15	ALA	N-CA-C	6.23	118.87	111.33
1	C	28	HIS	CB-CA-C	-6.22	101.03	110.92
1	D	128	LEU	N-CA-C	-6.22	99.11	109.24
1	A	192	SER	N-CA-CB	-6.21	100.73	110.30
1	D	136	LYS	O-C-N	6.21	130.69	123.17
1	A	65	ASN	N-CA-C	-6.20	104.63	111.82
1	C	129	GLY	CA-C-N	-6.19	114.27	122.99
1	C	129	GLY	C-N-CA	-6.19	114.27	122.99
1	D	48	GLU	CB-CA-C	-6.18	100.53	110.79
1	A	5	THR	O-C-N	6.18	130.29	123.25
1	B	128	LEU	CA-C-N	-6.17	116.64	121.82
1	B	128	LEU	C-N-CA	-6.17	116.64	121.82
1	C	72	GLY	CA-C-N	-6.17	110.93	120.31
1	C	72	GLY	C-N-CA	-6.17	110.93	120.31
1	D	110	ARG	CA-C-N	-6.17	110.17	121.52
1	D	110	ARG	C-N-CA	-6.17	110.17	121.52
1	C	103	PHE	CB-CA-C	-6.16	101.10	111.02
1	A	187	TRP	N-CA-C	6.16	120.40	113.01
1	B	44	VAL	CA-CB-CG1	-6.15	99.95	110.40
1	B	66	LEU	CA-C-N	-6.15	110.96	120.31
1	B	66	LEU	C-N-CA	-6.15	110.96	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	ASP	CA-C-N	-6.15	110.06	120.58
1	D	176	ASP	C-N-CA	-6.15	110.06	120.58
1	C	117	ALA	N-CA-CB	-6.14	101.05	110.20
1	B	125	TRP	N-CA-CB	-6.13	101.07	111.31
1	B	50	ALA	N-CA-CB	-6.13	100.86	110.30
1	C	59	ILE	CA-CB-CG2	6.13	120.92	110.50
1	B	130	TRP	CB-CA-C	6.13	120.32	109.72
1	C	179	LYS	CA-C-N	-6.12	110.49	120.72
1	C	179	LYS	C-N-CA	-6.12	110.49	120.72
1	B	93	GLY	N-CA-C	6.12	122.41	111.02
1	A	62	ASN	CA-C-N	-6.12	110.43	121.14
1	A	62	ASN	C-N-CA	-6.12	110.43	121.14
1	D	156	LEU	CA-C-N	-6.12	112.19	121.86
1	D	156	LEU	C-N-CA	-6.12	112.19	121.86
1	C	130	TRP	N-CA-CB	-6.12	100.40	110.68
1	A	41	ASN	N-CA-CB	6.11	118.88	110.01
1	D	76	HIS	O-C-N	6.11	128.37	122.07
1	B	84	SER	CA-C-N	6.11	126.56	119.47
1	B	84	SER	C-N-CA	6.11	126.56	119.47
1	C	112	GLN	N-CA-C	-6.10	103.95	111.40
1	D	38	LYS	CA-CB-CG	-6.10	101.90	114.10
1	A	73	HIS	N-CA-CB	-6.08	101.16	110.16
1	A	109	PHE	CA-CB-CG	-6.08	107.72	113.80
1	A	136	LYS	O-C-N	6.08	130.20	123.33
1	A	137	LEU	CA-C-N	-6.08	110.50	121.62
1	A	137	LEU	C-N-CA	-6.08	110.50	121.62
1	A	149	PHE	O-C-N	6.07	127.57	121.56
1	C	147	THR	OG1-CB-CG2	-6.07	97.16	109.30
1	B	85	PRO	CB-CA-C	-6.06	102.13	112.26
1	A	175	VAL	N-CA-CB	-6.06	98.05	111.50
1	A	33	HIS	N-CA-CB	-6.05	101.23	110.12
1	A	19	HIS	CA-CB-CG	-6.04	107.75	113.80
1	A	116	ALA	CA-C-N	-6.04	110.40	121.52
1	A	116	ALA	C-N-CA	-6.04	110.40	121.52
1	B	99	ILE	CB-CA-C	-6.04	103.97	111.70
1	C	136	LYS	CA-C-N	-6.04	114.67	123.00
1	C	136	LYS	C-N-CA	-6.04	114.67	123.00
1	C	178	ALA	N-CA-CB	-6.03	101.26	110.12
1	D	92	THR	CA-CB-CG2	6.03	120.75	110.50
1	A	196	ALA	N-CA-C	-6.03	104.28	111.69
1	A	3	GLU	CA-CB-CG	-6.01	102.07	114.10
1	B	154	VAL	CA-C-N	6.01	126.49	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	VAL	C-N-CA	6.01	126.49	119.99
1	C	148	ASN	N-CA-C	6.01	123.61	110.80
1	B	180	ALA	CB-CA-C	-6.01	100.63	110.85
1	C	36	TYR	N-CA-C	-6.01	104.64	111.07
1	B	153	ILE	CA-C-N	-6.00	116.78	123.02
1	B	153	ILE	C-N-CA	-6.00	116.78	123.02
1	A	56	HIS	CA-CB-CG	-6.00	107.80	113.80
1	A	90	LYS	CA-CB-CG	-6.00	102.09	114.10
1	C	162	TRP	N-CA-C	-6.00	101.40	110.28
1	C	68	PHE	CB-CA-C	5.99	120.29	110.88
1	B	103	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	183	ASN	CA-CB-CG	-5.99	106.61	112.60
1	B	172	ASN	CA-CB-CG	-5.99	106.61	112.60
1	C	33	HIS	N-CA-C	5.96	119.38	111.75
1	C	143	TYR	CA-CB-CG	5.95	124.61	113.90
1	A	64	LYS	CG-CD-CE	-5.94	97.64	111.30
1	A	129	GLY	N-CA-C	-5.93	102.44	111.10
1	A	44	VAL	CA-C-N	-5.93	110.61	120.68
1	A	44	VAL	C-N-CA	-5.93	110.61	120.68
1	B	137	LEU	CB-CA-C	-5.92	101.30	110.78
1	D	181	PHE	N-CA-CB	-5.92	101.18	110.06
1	D	7	PRO	CB-CA-C	-5.91	102.44	110.60
1	B	48	GLU	CA-CB-CG	5.91	125.92	114.10
1	B	20	ILE	CA-CB-CG1	5.90	120.43	110.40
1	B	46	LYS	CB-CA-C	-5.89	98.40	109.72
1	A	4	TYR	CA-C-N	-5.89	111.56	121.75
1	A	4	TYR	C-N-CA	-5.89	111.56	121.75
1	D	114	HIS	N-CA-CB	-5.89	101.15	110.28
1	A	145	GLU	N-CA-C	-5.88	98.27	110.80
1	D	74	VAL	CA-C-N	-5.88	111.38	120.31
1	D	74	VAL	C-N-CA	-5.88	111.38	120.31
1	D	35	THR	CA-C-N	-5.88	111.95	120.29
1	D	35	THR	C-N-CA	-5.88	111.95	120.29
1	A	114	HIS	CA-C-N	-5.86	112.47	120.44
1	A	114	HIS	C-N-CA	-5.86	112.47	120.44
1	A	44	VAL	CA-C-O	5.85	126.79	120.47
1	A	110	ARG	N-CA-C	5.85	118.44	111.71
1	C	164	HIS	N-CA-CB	-5.85	100.15	110.39
1	D	4	TYR	CA-C-O	-5.85	115.05	121.89
1	B	139	ILE	N-CA-CB	-5.84	98.02	111.81
1	D	106	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	142	VAL	CA-C-N	-5.83	114.47	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	VAL	C-N-CA	-5.83	114.47	122.93
1	C	174	LYS	N-CA-CB	5.83	118.47	110.01
1	A	70	LEU	CD1-CG-CD2	5.83	123.63	110.80
1	C	145	GLU	CA-CB-CG	5.83	125.76	114.10
1	D	162	TRP	CB-CG-CD2	-5.83	118.64	126.80
1	A	20	ILE	N-CA-C	-5.83	97.22	109.34
1	A	92	THR	CA-CB-OG1	-5.82	100.87	109.60
1	C	179	LYS	CA-CB-CG	-5.82	102.46	114.10
1	A	21	SER	N-CA-C	5.82	118.26	110.35
1	B	105	SER	N-CA-CB	-5.81	101.81	111.57
1	D	26	GLU	CA-CB-CG	-5.81	102.48	114.10
1	B	2	ALA	CB-CA-C	-5.81	101.79	110.50
1	A	74	VAL	N-CA-CB	-5.81	100.26	110.77
1	C	174	LYS	CB-CA-C	5.81	120.00	110.88
1	A	37	VAL	N-CA-CB	-5.80	101.87	110.58
1	D	29	HIS	N-CA-CB	-5.80	101.66	110.07
1	A	125	TRP	CA-C-N	-5.80	113.71	122.81
1	A	125	TRP	C-N-CA	-5.80	113.71	122.81
1	D	171	LYS	CA-CB-CG	-5.80	102.50	114.10
1	B	111	ALA	N-CA-CB	-5.79	101.38	110.30
1	C	29	HIS	CA-CB-CG	-5.79	108.01	113.80
1	C	176	ASP	N-CA-C	-5.79	106.21	113.28
1	D	61	LEU	N-CA-C	-5.79	105.31	112.90
1	B	73	HIS	CA-CB-CG	-5.79	108.01	113.80
1	B	58	ALA	N-CA-CB	-5.79	101.68	111.17
1	C	27	LEU	N-CA-C	-5.79	104.34	111.40
1	C	149	PHE	CA-C-N	-5.78	114.61	120.85
1	C	149	PHE	C-N-CA	-5.78	114.61	120.85
1	B	112	GLN	OE1-CD-NE2	5.77	128.37	122.60
1	A	37	VAL	CA-C-N	-5.77	112.94	120.44
1	A	37	VAL	C-N-CA	-5.77	112.94	120.44
1	A	5	THR	CB-CA-C	-5.76	98.06	110.45
1	D	11	TRP	CA-C-N	-5.76	112.21	122.07
1	D	11	TRP	C-N-CA	-5.76	112.21	122.07
1	B	3	GLU	CA-C-N	-5.75	111.91	120.94
1	B	3	GLU	C-N-CA	-5.75	111.91	120.94
1	C	144	ASP	CA-C-N	-5.75	113.18	121.98
1	C	144	ASP	C-N-CA	-5.75	113.18	121.98
1	D	85	PRO	N-CA-C	-5.73	105.72	113.40
1	B	46	LYS	CA-CB-CG	-5.73	102.65	114.10
1	B	79	TRP	N-CA-C	-5.73	104.49	112.45
1	A	36	TYR	N-CA-CB	-5.72	101.41	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ARG	CB-CA-C	5.72	119.94	110.90
1	A	88	GLY	N-CA-C	-5.71	104.17	112.17
1	C	161	MET	CA-C-N	-5.71	112.76	120.87
1	C	161	MET	C-N-CA	-5.71	112.76	120.87
1	A	38	LYS	N-CA-CB	-5.71	101.73	110.01
1	B	38	LYS	CA-CB-CG	-5.70	102.70	114.10
1	D	187	TRP	CA-C-N	-5.70	111.64	120.31
1	D	187	TRP	C-N-CA	-5.70	111.64	120.31
1	A	48	GLU	CB-CA-C	-5.70	101.94	110.88
1	C	47	LEU	N-CA-C	-5.70	105.05	112.23
1	A	118	THR	N-CA-C	5.70	120.23	113.28
1	C	66	LEU	N-CA-C	-5.69	104.69	111.69
1	B	125	TRP	CA-C-N	-5.68	114.69	122.93
1	B	125	TRP	C-N-CA	-5.68	114.69	122.93
1	B	110	ARG	N-CA-C	5.67	118.40	111.82
1	C	133	LEU	N-CA-C	-5.67	104.56	112.45
1	D	101	ASP	N-CA-C	-5.67	105.18	111.36
1	D	185	VAL	CA-C-N	-5.67	114.42	122.41
1	D	185	VAL	C-N-CA	-5.67	114.42	122.41
1	C	163	GLU	CA-C-O	5.67	126.75	120.63
1	D	146	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	B	64	LYS	N-CA-CB	-5.66	101.78	110.16
1	B	11	TRP	CB-CA-C	5.66	123.93	111.09
1	D	124	GLY	CA-C-O	-5.66	115.88	121.48
1	A	96	ALA	CB-CA-C	-5.66	100.17	110.63
1	B	125	TRP	CB-CG-CD1	5.66	135.38	126.90
1	D	40	ALA	CB-CA-C	-5.65	102.00	110.88
1	B	138	LEU	N-CA-CB	-5.65	101.72	111.55
1	C	92	THR	CA-CB-CG2	-5.65	100.89	110.50
1	B	66	LEU	N-CA-CB	-5.65	101.80	110.16
1	D	10	ASP	N-CA-CB	-5.65	103.07	111.43
1	B	194	TYR	CB-CA-C	5.65	119.75	110.88
1	C	103	PHE	CA-CB-CG	-5.65	108.15	113.80
1	B	16	LEU	N-CA-C	5.65	120.01	113.18
1	B	45	ALA	N-CA-C	5.64	118.36	111.82
1	B	69	ASN	N-CA-CB	-5.64	101.82	110.16
1	B	22	GLY	CA-C-N	-5.63	111.10	120.68
1	B	22	GLY	C-N-CA	-5.63	111.10	120.68
1	D	24	ILE	CA-CB-CG2	-5.63	100.92	110.50
1	B	116	ALA	CB-CA-C	-5.62	100.22	110.63
1	A	150	PRO	O-C-N	-5.62	116.41	123.21
1	B	51	ARG	N-CA-CB	-5.62	101.92	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ALA	CA-C-N	-5.62	112.99	120.63
1	A	97	ALA	C-N-CA	-5.62	112.99	120.63
1	C	77	THR	CA-CB-CG2	-5.62	100.95	110.50
1	C	135	ASN	CA-C-O	-5.61	115.33	121.84
1	D	138	LEU	O-C-N	5.60	130.44	123.15
1	B	63	GLU	CA-C-N	-5.60	112.33	120.29
1	B	63	GLU	C-N-CA	-5.60	112.33	120.29
1	C	19	HIS	N-CA-C	5.60	117.46	111.36
1	A	164	HIS	CA-C-N	-5.60	110.67	121.58
1	A	164	HIS	C-N-CA	-5.60	110.67	121.58
1	C	6	LEU	CA-C-N	-5.58	114.22	120.14
1	C	6	LEU	C-N-CA	-5.58	114.22	120.14
1	D	75	ASN	N-CA-CB	-5.58	101.64	110.28
1	C	10	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	55	ASP	CB-CA-C	-5.57	102.59	111.17
1	C	159	LEU	CB-CA-C	-5.55	102.24	110.62
1	C	63	GLU	N-CA-C	-5.55	105.38	111.82
1	A	191	GLN	N-CA-CB	-5.55	101.68	110.22
1	B	114	HIS	N-CA-C	-5.55	106.01	112.89
1	B	137	LEU	O-C-N	5.55	129.65	123.05
1	D	26	GLU	N-CA-C	5.55	117.41	111.36
1	B	46	LYS	N-CA-C	-5.54	106.52	113.28
1	D	109	PHE	O-C-N	5.54	127.78	122.07
1	A	175	VAL	N-CA-C	-5.53	104.81	112.50
1	C	31	LYS	CA-CB-CG	-5.53	103.04	114.10
1	A	10	ASP	CA-CB-CG	-5.52	107.08	112.60
1	A	101	ASP	N-CA-C	-5.52	106.38	113.23
1	B	144	ASP	CB-CA-C	-5.52	109.72	117.23
1	D	91	PRO	N-CA-C	-5.52	103.49	111.22
1	D	23	GLN	CA-C-N	-5.52	113.61	120.56
1	D	23	GLN	C-N-CA	-5.52	113.61	120.56
1	C	132	THR	CB-CA-C	-5.51	100.09	110.01
1	B	47	LEU	N-CA-CB	-5.50	101.99	110.13
1	D	161	MET	CG-SD-CE	5.49	112.98	100.90
1	C	56	HIS	CA-CB-CG	-5.49	108.31	113.80
1	D	34	ALA	CA-C-N	-5.49	112.92	120.28
1	D	34	ALA	C-N-CA	-5.49	112.92	120.28
1	A	139	ILE	N-CA-C	-5.48	100.56	108.89
1	D	60	LEU	CA-C-N	-5.48	111.44	121.52
1	D	60	LEU	C-N-CA	-5.48	111.44	121.52
1	A	48	GLU	N-CA-C	-5.47	105.22	111.07
1	A	117	ALA	N-CA-CB	-5.47	102.13	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	GLY	N-CA-C	-5.47	106.04	113.37
1	B	197	ALA	N-CA-CB	-5.46	101.81	110.28
1	A	137	LEU	N-CA-C	-5.46	100.79	109.96
1	D	33	HIS	N-CA-CB	-5.45	101.82	110.22
1	C	58	ALA	N-CA-CB	-5.45	102.30	110.91
1	B	61	LEU	N-CA-CB	-5.45	102.17	110.07
1	A	182	TRP	CA-C-O	5.45	125.96	119.10
1	D	82	ASN	CB-CA-C	-5.44	100.22	110.01
1	B	158	LEU	CB-CA-C	-5.44	98.01	109.38
1	B	45	ALA	CA-C-N	-5.43	111.96	122.06
1	B	45	ALA	C-N-CA	-5.43	111.96	122.06
1	B	114	HIS	N-CA-CB	-5.43	101.55	110.40
1	B	184	VAL	CA-CB-CG1	-5.43	101.17	110.40
1	A	103	PHE	CA-CB-CG	-5.43	108.37	113.80
1	D	116	ALA	CA-C-N	-5.43	112.11	121.66
1	D	116	ALA	C-N-CA	-5.43	112.11	121.66
1	D	139	ILE	CB-CA-C	-5.43	102.56	110.81
1	B	36	TYR	N-CA-C	-5.42	105.28	111.14
1	A	179	LYS	N-CA-C	-5.41	104.93	112.45
1	C	29	HIS	CB-CA-C	-5.41	102.62	110.96
1	A	176	ASP	N-CA-CB	-5.41	102.22	110.07
1	B	35	THR	CA-CB-CG2	-5.41	101.30	110.50
1	B	38	LYS	N-CA-CB	-5.41	101.97	110.30
1	A	62	ASN	N-CA-CB	-5.40	102.17	110.16
1	A	125	TRP	CB-CG-CD2	-5.40	119.24	126.80
1	C	24	ILE	CA-C-O	-5.40	115.45	121.17
1	A	103	PHE	CB-CA-C	-5.40	102.75	111.28
1	D	120	VAL	CA-CB-CG1	-5.40	101.22	110.40
1	D	149	PHE	N-CA-C	-5.39	103.36	108.22
1	A	36	TYR	N-CA-C	-5.39	105.57	111.82
1	B	60	LEU	CD1-CG-CD2	5.39	122.66	110.80
1	C	135	ASN	CB-CA-C	-5.39	104.24	111.89
1	D	158	LEU	N-CA-C	5.39	118.27	109.59
1	D	78	ILE	CB-CA-C	-5.39	103.38	112.16
1	C	11	TRP	CB-CA-C	5.39	120.64	110.62
1	C	142	VAL	N-CA-CB	-5.38	103.13	110.56
1	B	160	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	41	ASN	N-CA-CB	-5.38	101.94	110.22
1	D	153	ILE	CB-CA-C	-5.38	104.16	111.15
1	A	11	TRP	CA-C-N	-5.37	112.96	122.74
1	A	11	TRP	C-N-CA	-5.37	112.96	122.74
1	A	115	ALA	N-CA-CB	-5.37	102.28	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ALA	CA-C-N	-5.37	111.28	121.54
1	A	165	ALA	C-N-CA	-5.37	111.28	121.54
1	D	84	SER	N-CA-CB	5.37	118.23	110.77
1	A	26	GLU	CA-C-N	-5.37	111.75	121.14
1	A	26	GLU	C-N-CA	-5.37	111.75	121.14
1	C	8	ASP	CA-C-N	-5.37	113.38	122.67
1	C	8	ASP	C-N-CA	-5.37	113.38	122.67
1	C	19	HIS	CA-C-N	-5.37	114.98	122.71
1	C	19	HIS	C-N-CA	-5.37	114.98	122.71
1	B	73	HIS	N-CA-CB	-5.36	102.29	110.07
1	C	176	ASP	CA-C-O	5.36	125.56	119.18
1	A	178	ALA	CB-CA-C	-5.36	99.28	109.95
1	B	20	ILE	O-C-N	5.36	129.27	122.57
1	C	132	THR	N-CA-CB	-5.36	102.24	110.44
1	D	117	ALA	CB-CA-C	-5.36	98.68	109.55
1	D	89	ASP	N-CA-CB	-5.35	101.44	110.49
1	B	161	MET	CA-C-N	-5.34	110.10	121.32
1	B	161	MET	C-N-CA	-5.34	110.10	121.32
1	D	95	LEU	N-CA-C	5.34	117.52	111.11
1	B	138	LEU	CA-C-N	-5.34	114.67	122.68
1	B	138	LEU	C-N-CA	-5.34	114.67	122.68
1	C	20	ILE	CA-CB-CG2	5.34	119.58	110.50
1	C	157	LEU	N-CA-C	-5.34	98.95	108.13
1	C	61	LEU	CA-C-N	-5.33	112.20	120.31
1	C	61	LEU	C-N-CA	-5.33	112.20	120.31
1	C	131	ASP	N-CA-CB	-5.33	101.74	110.21
1	B	131	ASP	CA-CB-CG	-5.33	107.28	112.60
1	D	105	SER	N-CA-CB	-5.33	103.31	111.56
1	D	155	PRO	CA-C-O	-5.32	114.75	120.97
1	A	149	PHE	CA-C-O	-5.32	115.72	120.56
1	D	120	VAL	CG1-CB-CG2	-5.32	99.10	110.80
1	D	138	LEU	CA-C-N	5.32	129.96	123.10
1	D	138	LEU	C-N-CA	5.32	129.96	123.10
1	D	68	PHE	CB-CA-C	5.31	119.30	110.90
1	C	92	THR	N-CA-CB	-5.30	102.01	111.08
1	A	40	ALA	N-CA-C	-5.30	105.58	111.36
1	B	94	GLU	N-CA-CB	5.30	118.00	110.16
1	C	109	PHE	CA-C-O	-5.30	115.44	120.90
1	B	58	ALA	CB-CA-C	-5.29	102.62	111.13
1	D	123	SER	CB-CA-C	-5.29	101.08	109.80
1	A	171	LYS	CA-CB-CG	-5.28	103.55	114.10
1	B	146	GLN	CA-C-N	-5.28	112.51	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	GLN	C-N-CA	-5.28	112.51	121.85
1	C	77	THR	CA-CB-OG1	-5.27	101.69	109.60
1	A	20	ILE	CB-CA-C	-5.27	102.65	111.29
1	A	193	ARG	N-CA-CB	-5.27	102.11	110.28
1	B	145	GLU	N-CA-CB	-5.27	101.55	110.51
1	D	23	GLN	N-CA-CB	-5.27	102.43	110.07
1	D	14	GLY	CA-C-O	5.27	125.73	119.10
1	D	72	GLY	CA-C-O	5.26	126.09	120.30
1	B	168	LEU	CA-C-O	5.26	126.12	120.55
1	D	122	GLY	CA-C-N	-5.25	113.19	122.74
1	D	122	GLY	C-N-CA	-5.25	113.19	122.74
1	A	32	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	184	VAL	N-CA-CB	5.24	117.98	112.21
1	A	195	ALA	CA-C-N	-5.24	111.61	120.58
1	A	195	ALA	C-N-CA	-5.24	111.61	120.58
1	D	99	ILE	N-CA-C	5.24	118.41	111.17
1	B	144	ASP	CA-CB-CG	-5.24	107.36	112.60
1	C	113	PHE	N-CA-CB	-5.24	102.16	110.28
1	C	135	ASN	O-C-N	5.23	129.04	122.55
1	D	38	LYS	CB-CA-C	-5.23	101.95	110.85
1	C	148	ASN	CA-C-N	-5.23	114.54	122.07
1	C	148	ASN	C-N-CA	-5.23	114.54	122.07
1	D	142	VAL	CA-C-N	-5.23	115.35	122.93
1	D	142	VAL	C-N-CA	-5.23	115.35	122.93
1	A	38	LYS	CB-CA-C	5.22	119.08	110.88
1	C	162	TRP	N-CA-CB	-5.22	102.29	109.97
1	B	68	PHE	N-CA-CB	-5.22	102.51	110.07
1	C	194	TYR	N-CA-C	-5.21	105.66	112.23
1	A	109	PHE	CB-CA-C	-5.21	102.69	110.88
1	D	167	TYR	CA-CB-CG	-5.20	104.54	113.90
1	B	189	ASP	N-CA-C	-5.20	105.30	111.69
1	D	173	VAL	CG1-CB-CG2	-5.20	99.37	110.80
1	D	86	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	158	LEU	N-CA-CB	-5.19	102.66	111.69
1	A	34	ALA	CB-CA-C	-5.19	100.71	110.67
1	D	123	SER	N-CA-CB	-5.19	102.47	110.56
1	D	137	LEU	CB-CA-C	-5.18	102.49	110.78
1	B	118	THR	N-CA-C	5.18	119.58	113.16
1	B	147	THR	CA-CB-OG1	-5.18	101.84	109.60
1	A	25	ASN	CA-C-N	-5.17	111.73	120.58
1	A	25	ASN	C-N-CA	-5.17	111.73	120.58
1	B	90	LYS	N-CA-C	5.17	118.09	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	ALA	N-CA-CB	-5.17	102.26	110.22
1	A	151	LEU	CB-CA-C	-5.17	99.09	109.68
1	A	113	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	108	LYS	N-CA-CB	-5.16	102.40	110.44
1	B	148	ASN	N-CA-C	5.15	121.78	110.80
1	B	158	LEU	CD1-CG-CD2	-5.15	99.47	110.80
1	D	135	ASN	N-CA-CB	5.15	119.20	110.49
1	D	79	TRP	CA-C-N	-5.15	112.98	120.29
1	D	79	TRP	C-N-CA	-5.15	112.98	120.29
1	B	156	LEU	CA-C-N	-5.14	113.69	122.33
1	B	156	LEU	C-N-CA	-5.14	113.69	122.33
1	C	113	PHE	CA-C-N	-5.14	111.79	120.58
1	C	113	PHE	C-N-CA	-5.14	111.79	120.58
1	A	69	ASN	O-C-N	-5.14	116.29	122.15
1	A	142	VAL	CA-CB-CG1	5.14	119.13	110.40
1	C	114	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	110	ARG	N-CA-CB	-5.13	102.32	110.22
1	B	35	THR	OG1-CB-CG2	-5.13	99.04	109.30
1	A	77	THR	N-CA-CB	-5.13	102.58	110.12
1	A	83	LEU	CB-CA-C	-5.13	99.23	109.33
1	C	26	GLU	CA-C-N	-5.13	112.14	120.71
1	C	26	GLU	C-N-CA	-5.13	112.14	120.71
1	C	101	ASP	N-CA-CB	-5.13	102.54	110.13
1	D	65	ASN	CA-CB-CG	-5.13	107.47	112.60
1	C	21	SER	N-CA-CB	-5.13	103.03	110.36
1	B	169	GLN	CB-CG-CD	-5.12	103.89	112.60
1	D	21	SER	CB-CA-C	-5.12	100.45	109.62
1	C	31	LYS	CD-CE-NZ	-5.12	95.51	111.90
1	C	107	ASP	N-CA-CB	5.12	118.90	110.39
1	D	117	ALA	CA-C-O	5.12	125.26	119.27
1	A	93	GLY	CA-C-N	5.12	127.45	120.54
1	A	93	GLY	C-N-CA	5.12	127.45	120.54
1	A	65	ASN	CA-CB-CG	-5.11	107.49	112.60
1	B	119	THR	OG1-CB-CG2	-5.11	99.08	109.30
1	D	4	TYR	CA-CB-CG	-5.11	104.70	113.90
1	D	143	TYR	CA-C-N	-5.11	115.58	123.04
1	D	143	TYR	C-N-CA	-5.11	115.58	123.04
1	A	154	VAL	CA-C-N	-5.11	114.69	119.85
1	A	154	VAL	C-N-CA	-5.11	114.69	119.85
1	A	135	ASN	CB-CA-C	-5.10	102.91	112.30
1	B	190	VAL	CB-CA-C	5.10	119.26	112.22
1	D	55	ASP	CA-CB-CG	-5.10	107.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ILE	N-CA-C	-5.10	105.74	110.53
1	A	53	LYS	N-CA-CB	-5.09	102.61	110.46
1	A	66	LEU	CB-CA-C	-5.09	102.19	110.85
1	C	15	ALA	CA-C-N	-5.09	114.50	122.65
1	C	15	ALA	C-N-CA	-5.09	114.50	122.65
1	C	188	ALA	N-CA-CB	-5.09	102.63	110.16
1	B	19	HIS	N-CA-CB	-5.08	102.62	110.20
1	B	106	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	93	GLY	CA-C-N	5.08	127.04	120.44
1	C	93	GLY	C-N-CA	5.08	127.04	120.44
1	A	46	LYS	N-CA-C	-5.07	105.94	111.82
1	D	196	ALA	CB-CA-C	-5.07	100.03	110.38
1	D	138	LEU	N-CA-CB	-5.07	102.73	111.55
1	D	69	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	D	120	VAL	CB-CA-C	-5.07	103.56	111.26
1	B	78	ILE	CA-C-N	-5.06	110.86	121.64
1	B	78	ILE	C-N-CA	-5.06	110.86	121.64
1	D	29	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	157	LEU	N-CA-CB	-5.05	102.12	111.52
1	B	32	HIS	CA-C-N	-5.05	113.51	120.28
1	B	32	HIS	C-N-CA	-5.05	113.51	120.28
1	A	191	GLN	CA-C-N	-5.05	112.10	120.68
1	A	191	GLN	C-N-CA	-5.05	112.10	120.68
1	B	168	LEU	O-C-N	-5.05	116.77	122.12
1	C	181	PHE	CA-C-O	5.05	126.08	120.63
1	B	171	LYS	CB-CA-C	-5.04	110.74	116.54
1	D	176	ASP	N-CA-C	-5.04	106.39	112.54
1	B	162	TRP	CA-C-O	-5.04	115.87	121.81
1	A	86	ASN	CA-C-N	-5.03	116.74	122.83
1	A	86	ASN	C-N-CA	-5.03	116.74	122.83
1	B	12	ASP	N-CA-CB	-5.03	102.20	110.41
1	B	172	ASN	OD1-CG-ND2	5.03	127.63	122.60
1	B	119	THR	CB-CA-C	-5.03	102.92	111.02
1	C	160	ASP	CA-C-N	-5.03	114.67	122.67
1	C	160	ASP	C-N-CA	-5.03	114.67	122.67
1	D	20	ILE	CA-C-N	5.02	128.34	120.75
1	D	20	ILE	C-N-CA	5.02	128.34	120.75
1	B	61	LEU	CA-C-N	-5.02	113.55	120.28
1	B	61	LEU	C-N-CA	-5.02	113.55	120.28
1	B	130	TRP	O-C-N	-5.02	117.36	123.29
1	D	37	VAL	N-CA-CB	-5.02	101.68	110.77
1	C	34	ALA	N-CA-CB	-5.02	102.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	TRP	CB-CA-C	-5.01	99.71	111.09
1	D	192	SER	N-CA-CB	-5.01	102.51	110.28
1	A	10	ASP	N-CA-C	-5.01	107.66	112.97
1	A	125	TRP	CB-CG-CD1	5.01	134.41	126.90
1	C	69	ASN	CA-C-N	-5.00	113.18	120.29
1	C	69	ASN	C-N-CA	-5.00	113.18	120.29
1	D	108	LYS	CA-CB-CG	-5.00	104.10	114.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	20	ILE	CB
1	C	153	ILE	CB
1	D	161	MET	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1567	0	1488	44	0
1	B	1567	0	1488	45	0
1	C	1567	0	1488	54	0
1	D	1567	0	1488	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	70	0	0	1	0
3	B	81	0	0	0	0
3	C	69	0	0	5	0
3	D	68	0	0	3	0
All	All	6560	0	5952	182	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 15.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:GLY:O	1:C:89:ASP:HB2	1.39	1.07
1:B:95:LEU:HD21	1:B:190:VAL:HG12	1.41	1.02
1:A:88:GLY:O	1:A:89:ASP:HB2	1.66	0.92
1:C:88:GLY:O	1:C:89:ASP:CB	2.22	0.86
1:B:95:LEU:CD2	1:B:190:VAL:HG12	2.06	0.86
1:A:95:LEU:HD23	1:A:191:GLN:HG3	1.58	0.84
1:A:157:LEU:O	1:A:158:LEU:HD23	1.79	0.83
1:D:84:SER:OG	1:D:85:PRO:HD2	1.79	0.82
1:A:51:ARG:HG2	3:C:2039:HOH:O	1.82	0.78
1:D:146:GLN:N	1:D:146:GLN:OE1	2.17	0.78
1:C:84:SER:OG	1:C:85:PRO:HD2	1.84	0.77
1:D:88:GLY:O	1:D:89:ASP:HB2	1.87	0.74
1:B:64:LYS:HE3	3:D:2052:HOH:O	1.86	0.74
1:A:92:THR:CG2	1:A:93:GLY:N	2.49	0.74
1:B:27:LEU:O	1:B:31:LYS:HB2	1.88	0.74
1:C:64:LYS:HE3	3:C:2055:HOH:O	1.89	0.72
1:B:9:LEU:HD13	1:B:11:TRP:CZ3	2.25	0.72
1:C:63:GLU:HA	1:C:63:GLU:OE1	1.88	0.72
1:C:91:PRO:HD3	1:C:106:PHE:CE1	2.25	0.71
1:B:14:GLY:O	1:B:17:GLU:HG3	1.90	0.71
1:A:92:THR:HG22	1:A:93:GLY:N	1.94	0.71
1:D:92:THR:H	1:D:191:GLN:NE2	1.89	0.71
1:C:172:ASN:N	1:C:172:ASN:OD1	2.24	0.71
1:B:161:MET:HE1	1:B:174:LYS:HB2	1.71	0.70
1:C:92:THR:HG22	1:C:93:GLY:N	2.01	0.70
1:B:181:PHE:O	1:B:184:VAL:HG22	1.92	0.70
1:B:53:LYS:O	1:B:54:GLU:HB2	1.92	0.70
1:C:51:ARG:HG2	3:C:2027:HOH:O	1.92	0.69
1:A:95:LEU:HD22	1:A:191:GLN:HA	1.74	0.68
1:A:70:LEU:HD12	1:A:70:LEU:O	1.94	0.67
1:D:9:LEU:HD21	1:D:29:HIS:CD2	2.29	0.67
1:C:106:PHE:CE2	1:C:110:ARG:HD3	2.30	0.67
1:D:38:LYS:O	1:D:38:LYS:HG3	1.95	0.67
1:B:91:PRO:HG2	1:B:99:ILE:HD12	1.77	0.67
1:A:64:LYS:HE3	3:C:2056:HOH:O	1.96	0.66
1:C:170:TYR:O	1:C:173:VAL:HG23	1.95	0.65
1:C:92:THR:CG2	1:C:93:GLY:N	2.58	0.65
1:A:95:LEU:CD2	1:A:191:GLN:HG3	2.25	0.64
1:D:19:HIS:CE1	1:D:183:ASN:HD22	2.15	0.64
1:B:88:GLY:O	1:B:89:ASP:HB2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:HIS:O	1:C:37:VAL:HG23	1.98	0.63
1:D:95:LEU:HD21	1:D:190:VAL:HG12	1.80	0.62
1:B:51:ARG:HD3	1:D:112:GLN:OE1	1.99	0.62
1:C:169:GLN:HG2	1:C:170:TYR:CD2	2.35	0.61
1:B:95:LEU:HD21	1:B:190:VAL:CG1	2.27	0.59
1:D:9:LEU:HD21	1:D:29:HIS:HD2	1.66	0.59
1:C:64:LYS:HE2	1:D:121:GLN:OE1	2.03	0.59
1:D:146:GLN:H	1:D:146:GLN:CD	2.09	0.59
1:C:53:LYS:O	1:C:54:GLU:HB2	2.02	0.58
1:D:95:LEU:HD22	1:D:191:GLN:HA	1.85	0.57
1:C:146:GLN:O	1:C:146:GLN:HG2	2.04	0.57
1:D:64:LYS:O	1:D:64:LYS:HG3	2.05	0.57
1:C:14:GLY:O	1:C:17:GLU:HG2	2.05	0.56
1:A:147:THR:HG22	1:A:148:ASN:N	2.19	0.56
1:C:121:GLN:OE1	1:D:64:LYS:HE2	2.05	0.56
1:C:164:HIS:HB3	1:D:163:GLU:CD	2.30	0.56
1:B:9:LEU:HD21	1:B:29:HIS:CD2	2.40	0.56
1:B:83:LEU:HD22	1:B:184:VAL:HG23	1.87	0.56
1:A:186:ASN:OD1	1:A:186:ASN:C	2.47	0.55
1:A:95:LEU:HD22	1:A:191:GLN:CA	2.36	0.55
1:B:95:LEU:HD23	1:B:191:GLN:HG3	1.89	0.54
1:B:6:LEU:HD12	1:B:7:PRO:HD2	1.89	0.54
1:C:56:HIS:O	1:C:59:ILE:HG22	2.07	0.54
1:A:9:LEU:HD11	1:A:13:TYR:HE1	1.73	0.54
1:B:99:ILE:HG22	1:B:100:ALA:N	2.23	0.54
1:B:194:TYR:CE1	1:B:198:THR:HG21	2.42	0.54
1:A:147:THR:HG23	1:C:147:THR:OG1	2.08	0.53
1:D:90:LYS:HB3	1:D:91:PRO:HD2	1.90	0.53
1:B:9:LEU:CD1	1:B:11:TRP:CZ3	2.91	0.53
1:C:9:LEU:HD13	1:C:11:TRP:CZ3	2.43	0.53
1:A:63:GLU:HA	1:A:63:GLU:OE1	2.09	0.53
1:C:90:LYS:HB3	1:C:91:PRO:HD2	1.90	0.53
1:D:89:ASP:O	1:D:90:LYS:HG2	2.09	0.52
1:A:9:LEU:HD11	1:A:13:TYR:CE1	2.44	0.52
1:D:19:HIS:CE1	1:D:183:ASN:ND2	2.77	0.52
1:B:70:LEU:O	1:B:74:VAL:HG23	2.10	0.52
1:D:27:LEU:O	1:D:31:LYS:HB2	2.10	0.52
1:C:123:SER:HB3	1:C:162:TRP:CE2	2.44	0.52
1:D:130:TRP:CZ2	1:D:135:ASN:HB3	2.45	0.51
1:C:33:HIS:O	1:C:33:HIS:CD2	2.63	0.51
1:A:78:ILE:O	1:A:78:ILE:HG22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:TRP:CH2	1:D:16:LEU:HD11	2.46	0.50
1:C:147:THR:O	1:C:148:ASN:CB	2.59	0.50
1:B:19:HIS:CE1	1:B:183:ASN:HD22	2.29	0.50
1:A:146:GLN:OE1	1:A:146:GLN:N	2.40	0.50
1:B:161:MET:CE	1:B:174:LYS:HB2	2.40	0.50
1:A:84:SER:HB2	1:A:186:ASN:HB2	1.93	0.50
1:C:33:HIS:O	1:C:33:HIS:HD2	1.95	0.49
1:C:83:LEU:O	1:C:84:SER:HB2	2.11	0.49
1:D:14:GLY:O	1:D:17:GLU:HG3	2.12	0.49
1:D:88:GLY:O	1:D:89:ASP:CB	2.52	0.49
1:C:164:HIS:CD2	1:C:164:HIS:C	2.91	0.49
1:B:150:PRO:HD2	1:B:153:ILE:HG13	1.93	0.49
1:A:157:LEU:C	1:A:158:LEU:HD23	2.38	0.49
1:C:106:PHE:O	1:C:109:PHE:HB3	2.13	0.48
1:C:14:GLY:O	1:C:17:GLU:CG	2.61	0.48
1:B:97:ALA:O	1:B:101:ASP:HB2	2.14	0.48
1:D:84:SER:OG	1:D:85:PRO:CD	2.57	0.48
1:D:153:ILE:O	1:D:155:PRO:HD3	2.13	0.48
1:A:84:SER:OG	1:A:85:PRO:CD	2.62	0.48
1:A:169:GLN:NE2	1:A:170:TYR:CE2	2.82	0.48
1:B:92:THR:HG22	1:B:93:GLY:N	2.29	0.48
1:B:166:PHE:C	1:B:166:PHE:CD1	2.92	0.47
1:A:16:LEU:HB2	3:A:2015:HOH:O	2.15	0.47
1:A:147:THR:CG2	1:A:148:ASN:N	2.78	0.47
1:D:154:VAL:HA	1:D:155:PRO:HD2	1.69	0.47
1:C:42:ASP:HB3	3:C:2019:HOH:O	2.13	0.47
1:C:78:ILE:O	1:C:78:ILE:HG22	2.13	0.47
1:B:78:ILE:O	1:B:78:ILE:HG22	2.14	0.47
1:D:140:PHE:CE2	1:D:153:ILE:HD12	2.49	0.47
1:A:16:LEU:HD12	1:A:25:ASN:HD21	1.79	0.47
1:A:9:LEU:CD1	1:A:13:TYR:CE1	2.98	0.46
1:C:89:ASP:O	1:C:90:LYS:HG2	2.15	0.46
1:D:6:LEU:HA	1:D:7:PRO:HD2	1.82	0.46
1:A:137:LEU:O	1:A:138:LEU:HD23	2.16	0.46
1:C:91:PRO:CD	1:C:106:PHE:CE1	2.97	0.46
1:D:95:LEU:HD22	1:D:191:GLN:CA	2.46	0.46
1:A:63:GLU:OE1	1:A:63:GLU:CA	2.62	0.46
1:B:123:SER:HB3	1:B:162:TRP:CD2	2.51	0.45
1:B:153:ILE:HD13	1:B:153:ILE:HA	1.77	0.45
1:D:99:ILE:HD13	1:D:99:ILE:HG21	1.45	0.45
1:B:106:PHE:HE1	1:B:187:TRP:CZ2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LYS:C	1:C:83:LEU:H	2.23	0.45
1:D:36:TYR:CE2	1:D:76:HIS:CE1	3.04	0.45
1:C:104:GLY:O	1:C:105:SER:HB3	2.16	0.45
1:D:153:ILE:HD13	1:D:153:ILE:HG23	1.74	0.45
1:B:90:LYS:HB3	1:B:91:PRO:CD	2.47	0.45
1:B:171:LYS:HB3	1:B:172:ASN:H	1.65	0.45
1:A:49:GLU:O	1:A:53:LYS:HG3	2.17	0.45
1:C:84:SER:HA	1:C:85:PRO:HD3	1.86	0.44
1:B:9:LEU:HD13	1:B:11:TRP:CH2	2.52	0.44
1:C:13:TYR:O	1:C:22:GLY:HA2	2.17	0.44
1:A:112:GLN:O	1:A:115:ALA:HB3	2.18	0.44
1:C:71:ALA:O	1:C:72:GLY:C	2.60	0.44
1:D:186:ASN:ND2	1:D:189:ASP:HB2	2.33	0.44
1:D:131:ASP:O	1:D:135:ASN:HA	2.18	0.44
1:B:16:LEU:HD13	1:B:83:LEU:HD13	2.00	0.43
1:B:56:HIS:CE1	1:D:112:GLN:HG3	2.54	0.43
1:C:28:HIS:HB3	1:C:80:TRP:HH2	1.83	0.43
1:D:168:LEU:HA	1:D:168:LEU:HD23	1.66	0.43
1:C:110:ARG:HG3	1:C:182:TRP:CZ2	2.52	0.43
1:D:9:LEU:CD2	1:D:29:HIS:CD2	3.01	0.43
1:C:27:LEU:O	1:C:31:LYS:HB2	2.18	0.43
1:A:123:SER:HB3	1:A:162:TRP:CD2	2.54	0.43
1:B:60:LEU:C	1:B:60:LEU:HD13	2.43	0.43
1:A:19:HIS:CD2	1:A:183:ASN:HD22	2.37	0.43
1:D:143:TYR:O	1:D:144:ASP:HB2	2.19	0.43
1:A:189:ASP:O	1:A:192:SER:HB3	2.19	0.43
1:B:95:LEU:HB3	1:B:191:GLN:HG2	2.00	0.43
1:D:6:LEU:HD21	1:D:29:HIS:CE1	2.54	0.43
1:A:95:LEU:CB	1:A:191:GLN:HG2	2.49	0.42
1:B:143:TYR:HB2	1:B:147:THR:HB	2.01	0.42
1:A:64:LYS:O	1:A:64:LYS:HG3	2.20	0.42
1:B:118:THR:O	1:B:174:LYS:HE3	2.20	0.42
1:C:81:LYS:C	1:C:83:LEU:N	2.77	0.42
1:A:53:LYS:O	1:A:54:GLU:HB2	2.19	0.42
1:D:81:LYS:HE2	3:D:2031:HOH:O	2.18	0.42
1:A:95:LEU:CD2	1:A:191:GLN:CG	2.97	0.42
1:B:106:PHE:CE1	1:B:187:TRP:CZ2	3.07	0.42
1:D:40:ALA:N	1:D:69:ASN:HB3	2.35	0.42
1:D:36:TYR:HE2	1:D:76:HIS:CE1	2.38	0.41
1:C:137:LEU:CD2	1:C:156:LEU:CD1	2.98	0.41
1:D:75:ASN:HB3	1:D:125:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD13	1:B:60:LEU:O	2.20	0.41
1:D:91:PRO:HG2	3:D:2033:HOH:O	2.20	0.41
1:A:6:LEU:HA	1:A:6:LEU:HD12	1.85	0.41
1:B:11:TRP:CD1	1:B:85:PRO:HD3	2.55	0.41
1:C:174:LYS:O	1:C:177:PHE:HB3	2.20	0.41
1:A:147:THR:HG23	1:C:147:THR:HG23	2.03	0.41
1:C:103:PHE:CE1	1:C:139:ILE:HD12	2.55	0.41
1:C:104:GLY:O	1:C:105:SER:CB	2.68	0.41
1:D:149:PHE:HA	1:D:150:PRO:HD3	1.88	0.41
1:B:9:LEU:N	1:B:9:LEU:HD23	2.34	0.41
1:C:78:ILE:O	1:C:78:ILE:CG2	2.68	0.41
1:C:95:LEU:HA	1:C:95:LEU:HD12	1.77	0.41
1:A:67:ALA:O	1:A:71:ALA:HB2	2.21	0.40
1:C:109:PHE:HB3	1:C:110:ARG:H	1.66	0.40
1:C:6:LEU:HA	1:C:7:PRO:HD2	1.93	0.40
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.84	0.40
1:A:125:TRP:CE3	1:A:158:LEU:HB3	2.56	0.40
1:A:173:VAL:O	1:A:176:ASP:HB2	2.21	0.40
1:B:110:ARG:HH11	1:B:110:ARG:HD2	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/207 (95%)	177 (90%)	17 (9%)	2 (1%)	12	24
1	B	196/207 (95%)	184 (94%)	10 (5%)	2 (1%)	12	24
1	C	196/207 (95%)	175 (89%)	20 (10%)	1 (0%)	24	43
1	D	196/207 (95%)	182 (93%)	12 (6%)	2 (1%)	12	24
All	All	784/828 (95%)	718 (92%)	59 (8%)	7 (1%)	14	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	ASP
1	A	89	ASP
1	B	148	ASN
1	D	148	ASN
1	B	166	PHE
1	D	13	TYR
1	A	173	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/163 (96%)	133 (85%)	23 (15%)	3	6
1	B	156/163 (96%)	141 (90%)	15 (10%)	8	17
1	C	156/163 (96%)	141 (90%)	15 (10%)	8	17
1	D	156/163 (96%)	139 (89%)	17 (11%)	6	13
All	All	624/652 (96%)	554 (89%)	70 (11%)	6	12

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	17	GLU
1	A	21	SER
1	A	37	VAL
1	A	38	LYS
1	A	48	GLU
1	A	53	LYS
1	A	60	LEU
1	A	64	LYS
1	A	78	ILE
1	A	81	LYS
1	A	92	THR
1	A	99	ILE

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Mol	Chain	Res	Type
1	A	110	ARG
1	A	137	LEU
1	A	144	ASP
1	A	153	ILE
1	A	159	LEU
1	A	171	LYS
1	A	173	VAL
1	A	179	LYS
1	A	198	THR
1	A	199	SER
1	B	11	TRP
1	B	21	SER
1	B	48	GLU
1	B	51	ARG
1	B	53	LYS
1	B	64	LYS
1	B	74	VAL
1	B	82	ASN
1	B	83	LEU
1	B	99	ILE
1	B	101	ASP
1	B	105	SER
1	B	171	LYS
1	B	190	VAL
1	B	199	SER
1	C	20	ILE
1	C	21	SER
1	C	30	SER
1	C	46	LYS
1	C	48	GLU
1	C	49	GLU
1	C	64	LYS
1	C	137	LEU
1	C	139	ILE
1	C	150	PRO
1	C	159	LEU
1	C	164	HIS
1	C	167	TYR
1	C	173	VAL
1	C	199	SER
1	D	38	LYS
1	D	48	GLU

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Mol	Chain	Res	Type
1	D	53	LYS
1	D	59	ILE
1	D	60	LEU
1	D	64	LYS
1	D	77	THR
1	D	78	ILE
1	D	89	ASP
1	D	109	PHE
1	D	110	ARG
1	D	146	GLN
1	D	151	LEU
1	D	153	ILE
1	D	161	MET
1	D	173	VAL
1	D	179	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	69	ASN
1	A	183	ASN
1	B	19	HIS
1	B	23	GLN
1	B	56	HIS
1	B	82	ASN
1	B	114	HIS
1	B	148	ASN
1	B	186	ASN
1	C	19	HIS
1	C	56	HIS
1	C	62	ASN
1	C	135	ASN
1	D	19	HIS
1	D	29	HIS
1	D	62	ASN
1	D	183	ASN
1	D	186	ASN
1	D	191	GLN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/207 (95%)	-0.85	0 100 100	4, 20, 49, 89	0
1	B	198/207 (95%)	-0.65	0 100 100	7, 27, 61, 86	0
1	C	198/207 (95%)	-0.79	0 100 100	5, 20, 53, 84	0
1	D	198/207 (95%)	-0.74	0 100 100	7, 23, 57, 110	0
All	All	792/828 (95%)	-0.76	0 100 100	4, 22, 56, 110	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	B	1200	1/1	0.97	0.02	17,17,17,17	0
2	MN	A	1200	1/1	0.99	0.05	13,13,13,13	0
2	MN	C	1200	1/1	0.99	0.04	18,18,18,18	0
2	MN	D	1200	1/1	0.99	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.