



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 AM UTC

PDB ID : 2GDG / pdb_00002gdg
Title : Crystal structure of covalently modified macrophage inhibitory factor
Authors : Golubkov, P.A.; Hackert, M.L.
Deposited on : 2006-03-16
Resolution : 1.45 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

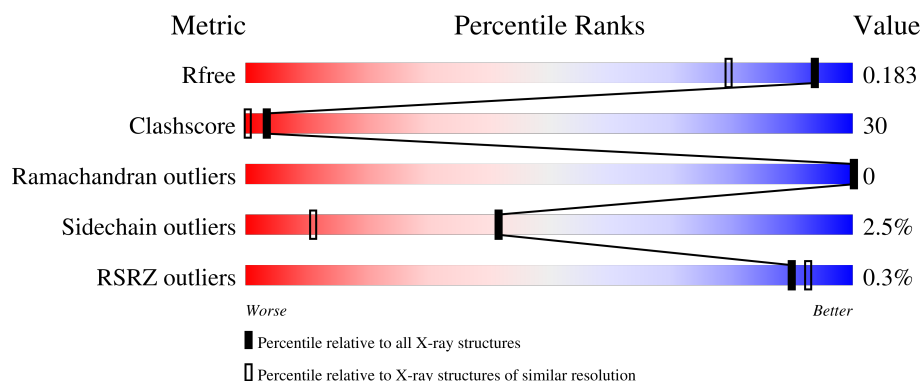
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

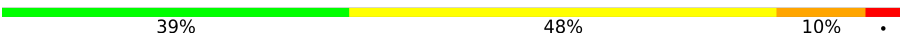
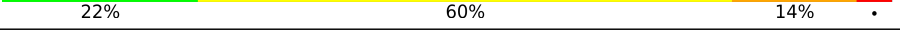
The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	114	
1	B	114	
1	C	114	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3072 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 Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			869	548	151	164	6			
1	B	114	Total	C	N	O	S	0	0	0
			869	548	151	164	6			
1	C	114	Total	C	N	O	S	0	0	0
			869	548	151	164	6			

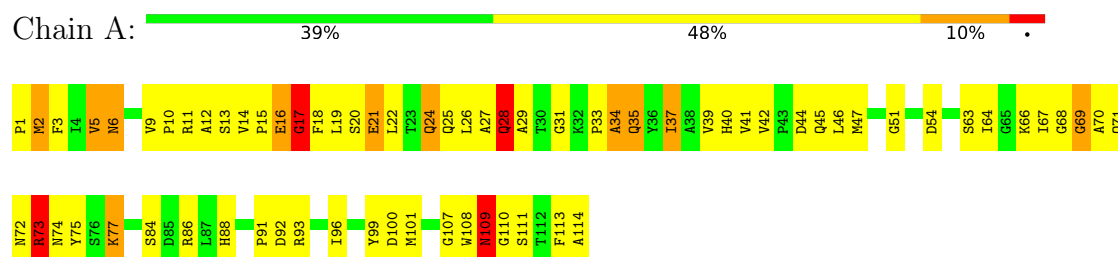
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	170	Total	O	0	0
			170	170		
2	B	159	Total	O	0	0
			159	159		
2	C	136	Total	O	0	0
			136	136		

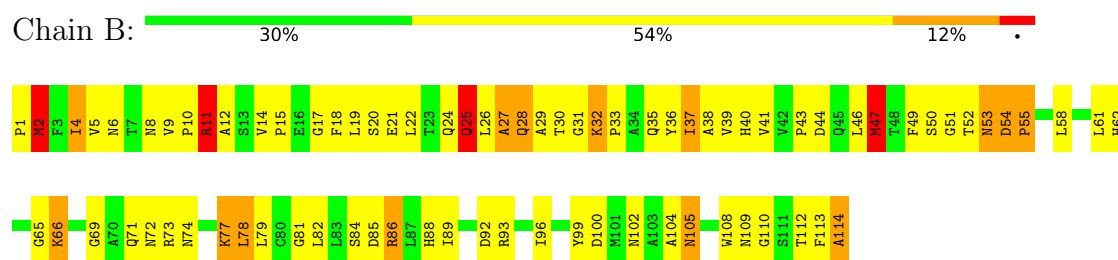
3 Residue-property plots

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.

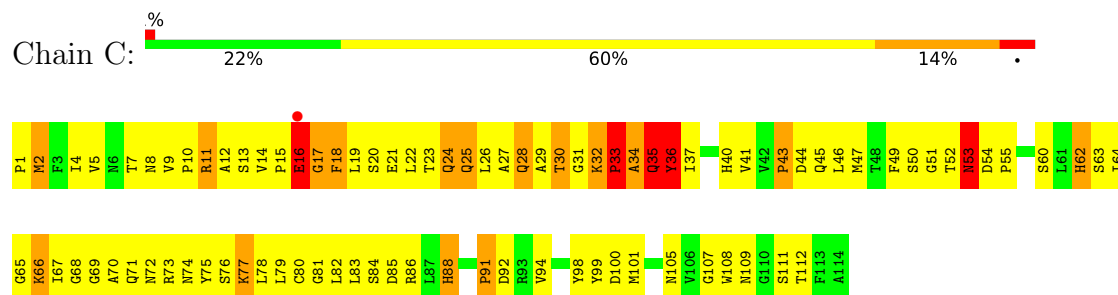
- Molecule 1: Macrophage migration inhibitory factor



- Molecule 1: Macrophage migration inhibitory factor



- Molecule 1: Macrophage migration inhibitory factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	94.70Å 94.70Å 87.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.45 50.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-1.45) 97.4 (50.00-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.147 , 0.183 0.147 , 0.183	Depositor DCC
R_{free} test set	3872 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3072	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

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	3.90	116/889 (13.0%)	3.29	107/1209 (8.9%)
1	B	5.02	142/889 (16.0%)	3.52	128/1209 (10.6%)
1	C	6.18	186/889 (20.9%)	4.53	193/1209 (16.0%)
All	All	5.11	444/2667 (16.6%)	3.82	428/3627 (11.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
1	C	0	10
All	All	0	19

All (444) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	GLU	CD-OE1	78.85	2.75	1.25
1	B	11	ARG	CZ-NH2	71.25	2.26	1.33
1	C	16	GLU	CA-C	51.53	2.15	1.52
1	C	16	GLU	CA-CB	49.45	2.20	1.53
1	C	16	GLU	CG-CD	40.55	2.53	1.52
1	C	11	ARG	CZ-NH2	34.98	1.78	1.33
1	B	66	LYS	CG-CD	-29.87	0.62	1.52
1	A	28	GLN	CD-OE1	29.05	1.78	1.23
1	C	88	HIS	CD2-NE2	28.62	1.69	1.37
1	C	53	ASN	CG-ND2	26.31	1.88	1.33
1	B	11	ARG	CD-NE	26.01	1.82	1.46
1	B	25	GLN	CD-NE2	25.28	1.86	1.33
1	B	11	ARG	CZ-NH1	24.92	1.67	1.32
1	A	28	GLN	CD-NE2	24.33	1.84	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	ARG	NE-CZ	22.38	1.57	1.33
1	A	73	ARG	NE-CZ	21.52	1.56	1.33
1	B	47	MET	SD-CE	-20.48	1.28	1.79
1	B	25	GLN	CD-OE1	19.49	1.60	1.23
1	C	36	TYR	CE2-CZ	18.96	1.83	1.38
1	A	17	GLY	N-CA	18.89	1.75	1.44
1	C	16	GLU	C-O	18.72	1.47	1.24
1	C	30	THR	C-N	-18.52	1.07	1.33
1	B	2	MET	CB-CG	-18.11	0.98	1.52
1	B	52	THR	C-O	17.64	1.46	1.23
1	C	11	ARG	CD-NE	17.46	1.70	1.46
1	A	73	ARG	CZ-NH1	17.04	1.56	1.32
1	C	53	ASN	CB-CG	-16.77	1.10	1.52
1	C	34	ALA	C-O	16.41	1.45	1.24
1	C	31	GLY	C-O	16.39	1.48	1.24
1	C	16	GLU	CD-OE2	16.38	1.56	1.25
1	C	35	GLN	CA-CB	16.25	1.79	1.53
1	C	17	GLY	CA-C	16.12	1.74	1.51
1	B	77	LYS	CE-NZ	15.93	1.97	1.49
1	A	16	GLU	CA-CB	15.71	1.79	1.53
1	C	36	TYR	CZ-OH	15.59	1.70	1.38
1	B	28	GLN	CD-NE2	15.15	1.65	1.33
1	B	66	LYS	CD-CE	15.14	1.97	1.52
1	B	54	ASP	CA-C	15.01	1.73	1.53
1	C	32	LYS	CA-CB	14.74	1.78	1.53
1	C	32	LYS	CE-NZ	14.59	1.93	1.49
1	A	86	ARG	CZ-NH1	14.44	1.52	1.32
1	B	29	ALA	C-O	14.37	1.42	1.24
1	C	34	ALA	CA-C	-14.29	1.33	1.52
1	C	15	PRO	N-CA	14.18	1.64	1.47
1	C	88	HIS	CE1-NE2	-14.09	1.18	1.32
1	B	114	ALA	C-OXT	13.98	1.51	1.23
1	C	88	HIS	CG-ND1	-13.75	1.23	1.38
1	A	35	GLN	CD-OE1	13.68	1.49	1.23
1	C	36	TYR	CD1-CE1	13.60	1.79	1.38
1	A	25	GLN	CD-NE2	13.53	1.61	1.33
1	B	25	GLN	CB-CG	13.43	1.92	1.52
1	C	36	TYR	CE1-CZ	13.43	1.70	1.38
1	B	28	GLN	CD-OE1	13.41	1.49	1.23
1	B	30	THR	C-O	13.19	1.41	1.24
1	B	32	LYS	CD-CE	13.08	1.91	1.52
1	C	86	ARG	CZ-NH2	12.98	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	MET	SD-CE	12.91	2.11	1.79
1	C	27	ALA	CA-CB	12.80	1.74	1.53
1	A	16	GLU	CG-CD	12.62	1.83	1.52
1	C	17	GLY	N-CA	12.54	1.63	1.45
1	B	88	HIS	CA-CB	12.53	1.73	1.53
1	C	24	GLN	CA-CB	12.44	1.74	1.53
1	A	16	GLU	CD-OE1	12.39	1.48	1.25
1	A	27	ALA	N-CA	12.38	1.61	1.46
1	C	28	GLN	CD-NE2	12.33	1.59	1.33
1	A	20	SER	CA-C	-12.28	1.36	1.52
1	C	35	GLN	CD-OE1	12.16	1.46	1.23
1	C	2	MET	CB-CG	-12.09	1.16	1.52
1	A	2	MET	SD-CE	-12.00	1.49	1.79
1	A	24	GLN	CG-CD	12.00	1.82	1.52
1	C	12	ALA	C-O	11.94	1.39	1.24
1	A	12	ALA	CA-C	-11.85	1.36	1.52
1	B	24	GLN	C-O	11.79	1.39	1.24
1	C	71	GLN	CD-NE2	11.61	1.57	1.33
1	A	86	ARG	NE-CZ	-11.53	1.20	1.33
1	A	24	GLN	CD-OE1	11.48	1.45	1.23
1	C	85	ASP	C-O	11.48	1.37	1.24
1	B	27	ALA	C-O	11.46	1.38	1.24
1	C	33	PRO	C-N	-11.32	1.16	1.33
1	C	81	GLY	C-O	11.31	1.37	1.23
1	A	113	PHE	C-O	11.28	1.39	1.24
1	C	24	GLN	CD-NE2	11.12	1.56	1.33
1	A	21	GLU	CG-CD	11.07	1.79	1.52
1	C	32	LYS	CG-CD	-11.01	1.19	1.52
1	A	2	MET	CG-SD	10.91	2.08	1.80
1	B	25	GLN	CG-CD	-10.84	1.25	1.52
1	B	50	SER	CA-C	-10.84	1.37	1.53
1	B	84	SER	C-O	10.72	1.36	1.24
1	C	14	VAL	CA-C	10.50	1.64	1.52
1	A	35	GLN	CG-CD	10.44	1.78	1.52
1	B	113	PHE	C-O	10.43	1.37	1.24
1	C	36	TYR	CB-CG	10.37	1.74	1.51
1	C	33	PRO	N-CD	10.37	1.62	1.47
1	A	88	HIS	CD2-NE2	10.35	1.49	1.37
1	A	28	GLN	CA-C	-10.26	1.39	1.52
1	A	73	ARG	CD-NE	-10.25	1.31	1.46
1	A	15	PRO	CA-C	-10.22	1.39	1.52
1	C	11	ARG	CZ-NH1	10.20	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	VAL	C-N	10.18	1.45	1.33
1	C	17	GLY	C-N	-10.15	1.20	1.34
1	B	33	PRO	C-O	10.13	1.35	1.23
1	A	15	PRO	N-CA	10.10	1.59	1.47
1	C	12	ALA	CA-C	-10.08	1.38	1.52
1	C	77	LYS	CA-C	-10.05	1.40	1.52
1	B	52	THR	CA-C	-9.98	1.40	1.52
1	A	35	GLN	CA-CB	9.97	1.71	1.53
1	C	36	TYR	CG-CD1	9.89	1.60	1.39
1	A	73	ARG	CZ-NH2	9.87	1.46	1.33
1	C	33	PRO	CA-CB	9.86	1.67	1.53
1	C	85	ASP	CG-OD2	9.84	1.44	1.25
1	C	82	LEU	C-N	9.83	1.47	1.34
1	B	51	GLY	C-N	-9.82	1.19	1.33
1	B	51	GLY	C-O	9.81	1.38	1.24
1	A	2	MET	CB-CG	-9.75	1.23	1.52
1	B	27	ALA	C-N	-9.71	1.21	1.33
1	A	11	ARG	CZ-NH1	9.66	1.46	1.32
1	C	88	HIS	ND1-CE1	9.64	1.42	1.32
1	B	32	LYS	CA-CB	9.51	1.68	1.53
1	B	82	LEU	C-O	9.46	1.35	1.24
1	C	85	ASP	CA-C	-9.36	1.40	1.52
1	C	28	GLN	CD-OE1	9.34	1.41	1.23
1	C	22	LEU	CA-C	9.30	1.64	1.52
1	C	69	GLY	C-O	-9.10	1.11	1.23
1	C	52	THR	C-O	9.09	1.35	1.23
1	C	2	MET	SD-CE	-9.04	1.56	1.79
1	A	15	PRO	C-N	9.03	1.45	1.33
1	C	88	HIS	CG-CD2	-9.01	1.25	1.35
1	A	12	ALA	C-O	8.96	1.35	1.24
1	C	30	THR	N-CA	8.93	1.57	1.46
1	C	67	ILE	C-O	8.91	1.33	1.24
1	C	26	LEU	N-CA	8.89	1.57	1.46
1	C	73	ARG	NE-CZ	8.88	1.42	1.33
1	A	31	GLY	N-CA	8.81	1.58	1.45
1	C	30	THR	CA-CB	-8.78	1.38	1.53
1	A	11	ARG	CD-NE	8.77	1.58	1.46
1	B	86	ARG	CA-C	-8.74	1.41	1.53
1	A	12	ALA	N-CA	8.71	1.57	1.46
1	B	12	ALA	CA-C	-8.71	1.40	1.52
1	A	9	VAL	CA-C	8.68	1.62	1.52
1	B	29	ALA	N-CA	8.66	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	GLY	C-N	8.64	1.46	1.33
1	B	54	ASP	CA-CB	8.64	1.65	1.53
1	B	79	LEU	C-O	8.63	1.34	1.24
1	C	77	LYS	N-CA	8.63	1.56	1.46
1	B	14	VAL	N-CA	8.61	1.53	1.46
1	B	78	LEU	CG-CD1	8.55	1.80	1.52
1	B	50	SER	CA-CB	8.54	1.66	1.53
1	B	93	ARG	N-CA	8.53	1.56	1.46
1	C	23	THR	CA-C	-8.48	1.42	1.52
1	B	78	LEU	C-O	8.45	1.33	1.24
1	C	50	SER	C-O	8.41	1.35	1.23
1	A	15	PRO	N-CD	8.40	1.59	1.47
1	A	14	VAL	N-CA	8.29	1.52	1.46
1	B	50	SER	C-O	8.29	1.35	1.23
1	C	66	LYS	CA-C	8.29	1.64	1.53
1	B	29	ALA	CA-C	-8.27	1.41	1.52
1	B	36	TYR	CZ-OH	8.26	1.55	1.38
1	A	2	MET	CA-CB	-8.24	1.39	1.53
1	C	100	ASP	CA-C	8.24	1.63	1.52
1	B	89	ILE	CA-C	8.19	1.62	1.52
1	C	33	PRO	N-CA	8.18	1.57	1.47
1	C	77	LYS	CD-CE	8.18	1.76	1.52
1	C	44	ASP	CB-CG	8.18	1.72	1.52
1	A	111	SER	CA-CB	8.16	1.64	1.53
1	B	88	HIS	CG-ND1	-8.15	1.29	1.38
1	B	62	HIS	ND1-CE1	8.14	1.40	1.32
1	C	20	SER	CA-C	-8.14	1.42	1.52
1	A	25	GLN	N-CA	-8.14	1.36	1.46
1	B	53	ASN	CA-CB	8.14	1.64	1.53
1	A	18	PHE	N-CA	8.07	1.56	1.46
1	B	28	GLN	CG-CD	8.05	1.72	1.52
1	C	81	GLY	CA-C	-8.03	1.43	1.52
1	C	24	GLN	CG-CD	8.01	1.72	1.52
1	C	66	LYS	CA-CB	-7.93	1.41	1.53
1	C	27	ALA	C-O	7.91	1.33	1.24
1	A	19	LEU	C-N	7.87	1.44	1.34
1	B	77	LYS	C-O	7.87	1.33	1.24
1	A	20	SER	CA-CB	7.85	1.66	1.53
1	C	13	SER	CB-OG	7.78	1.57	1.42
1	B	79	LEU	CA-C	-7.75	1.42	1.52
1	B	35	GLN	CA-CB	7.74	1.65	1.53
1	C	109	ASN	CG-ND2	-7.73	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	PHE	C-O	7.73	1.32	1.23
1	C	7	THR	N-CA	7.73	1.55	1.45
1	B	53	ASN	CB-CG	-7.67	1.32	1.52
1	B	12	ALA	N-CA	7.64	1.56	1.46
1	A	73	ARG	CG-CD	7.64	1.75	1.52
1	C	85	ASP	N-CA	7.63	1.55	1.46
1	C	1	PRO	N-CD	-7.63	1.37	1.47
1	B	102	ASN	CG-ND2	7.59	1.49	1.33
1	B	12	ALA	CA-CB	7.58	1.66	1.53
1	C	25	GLN	CB-CG	7.58	1.75	1.52
1	C	65	GLY	C-N	-7.57	1.23	1.33
1	B	11	ARG	CB-CG	-7.56	1.29	1.52
1	A	77	LYS	CE-NZ	7.56	1.72	1.49
1	B	8	ASN	C-O	7.55	1.34	1.24
1	C	10	PRO	CA-CB	7.51	1.63	1.53
1	C	22	LEU	CA-CB	7.48	1.65	1.53
1	A	19	LEU	CA-C	-7.47	1.43	1.52
1	B	114	ALA	C-O	7.43	1.38	1.23
1	C	36	TYR	CD2-CE2	7.40	1.60	1.38
1	B	25	GLN	C-N	-7.39	1.23	1.33
1	C	64	ILE	N-CA	7.37	1.55	1.46
1	A	113	PHE	CG-CD1	7.37	1.54	1.38
1	A	68	GLY	CA-C	-7.34	1.42	1.51
1	C	35	GLN	CD-NE2	7.34	1.48	1.33
1	C	33	PRO	C-O	-7.32	1.14	1.24
1	C	15	PRO	CA-CB	-7.31	1.43	1.53
1	B	1	PRO	CA-CB	-7.24	1.39	1.53
1	B	114	ALA	N-CA	7.24	1.60	1.46
1	C	60	SER	CA-CB	7.23	1.66	1.53
1	A	34	ALA	CA-CB	7.22	1.65	1.53
1	B	40	HIS	C-N	7.20	1.42	1.33
1	C	33	PRO	CG-CD	7.19	1.75	1.50
1	B	88	HIS	ND1-CE1	7.13	1.39	1.32
1	C	11	ARG	C-N	7.10	1.43	1.33
1	C	65	GLY	C-O	7.10	1.35	1.23
1	A	46	LEU	CA-C	7.09	1.61	1.52
1	B	50	SER	N-CA	7.08	1.57	1.46
1	C	88	HIS	CB-CG	7.06	1.60	1.50
1	A	37	ILE	CG1-CD1	-7.05	1.24	1.51
1	B	35	GLN	CD-OE1	7.04	1.36	1.23
1	B	54	ASP	C-N	-7.04	1.24	1.33
1	C	23	THR	C-N	7.03	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	ARG	CZ-NH1	7.03	1.42	1.32
1	C	109	ASN	C-O	7.03	1.32	1.23
1	C	62	HIS	CG-CD2	7.00	1.43	1.35
1	B	47	MET	CB-CG	-6.98	1.31	1.52
1	A	13	SER	CB-OG	6.97	1.56	1.42
1	B	82	LEU	CA-C	-6.97	1.43	1.52
1	A	110	GLY	C-N	-6.95	1.25	1.33
1	C	109	ASN	CG-OD1	6.95	1.36	1.23
1	C	9	VAL	N-CA	6.94	1.55	1.46
1	B	31	GLY	CA-C	-6.93	1.42	1.51
1	B	88	HIS	CD2-NE2	6.93	1.45	1.37
1	A	17	GLY	CA-C	-6.92	1.42	1.51
1	B	49	PHE	CD1-CE1	6.92	1.59	1.38
1	A	71	GLN	CD-OE1	6.91	1.36	1.23
1	A	67	ILE	C-O	6.90	1.31	1.24
1	C	60	SER	N-CA	6.90	1.54	1.46
1	C	111	SER	CA-C	-6.89	1.44	1.53
1	B	30	THR	CA-C	-6.88	1.43	1.52
1	C	67	ILE	CA-CB	6.87	1.63	1.54
1	B	66	LYS	CB-CG	6.86	1.73	1.52
1	A	47	MET	CA-C	-6.85	1.44	1.52
1	C	2	MET	CG-SD	6.82	1.97	1.80
1	C	15	PRO	CA-C	-6.82	1.43	1.52
1	C	2	MET	CA-C	-6.80	1.44	1.52
1	B	25	GLN	CA-C	6.77	1.61	1.52
1	C	50	SER	C-N	-6.77	1.24	1.33
1	C	47	MET	CA-C	-6.76	1.44	1.52
1	B	40	HIS	CE1-NE2	6.74	1.39	1.32
1	C	78	LEU	CA-C	-6.73	1.44	1.52
1	B	79	LEU	CA-CB	6.72	1.64	1.53
1	C	29	ALA	CA-CB	6.72	1.64	1.53
1	B	36	TYR	CE1-CZ	-6.68	1.22	1.38
1	C	15	PRO	C-N	6.67	1.42	1.33
1	A	20	SER	C-O	6.67	1.32	1.24
1	A	41	VAL	C-O	6.67	1.31	1.24
1	B	36	TYR	CE2-CZ	6.67	1.54	1.38
1	C	36	TYR	CG-CD2	6.67	1.53	1.39
1	B	77	LYS	CB-CG	6.66	1.72	1.52
1	C	73	ARG	CZ-NH1	6.66	1.42	1.32
1	C	54	ASP	CG-OD1	-6.64	1.12	1.25
1	A	109	ASN	CG-ND2	-6.63	1.19	1.33
1	C	21	GLU	N-CA	-6.63	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	VAL	CA-CB	6.60	1.62	1.54
1	B	77	LYS	N-CA	6.59	1.54	1.46
1	A	14	VAL	CA-C	-6.55	1.48	1.53
1	C	18	PHE	CA-C	6.49	1.61	1.52
1	C	41	VAL	CA-CB	6.49	1.62	1.54
1	B	85	ASP	C-O	6.48	1.31	1.24
1	B	88	HIS	C-N	6.48	1.46	1.33
1	C	76	SER	N-CA	6.45	1.54	1.46
1	B	33	PRO	CA-CB	6.45	1.62	1.53
1	A	88	HIS	CG-CD2	-6.44	1.28	1.35
1	B	5	VAL	CA-CB	6.44	1.62	1.54
1	B	19	LEU	CA-C	-6.43	1.44	1.52
1	B	77	LYS	CD-CE	-6.43	1.33	1.52
1	B	38	ALA	CA-C	-6.41	1.44	1.52
1	B	55	PRO	CA-CB	-6.39	1.45	1.53
1	B	10	PRO	CA-CB	6.38	1.62	1.53
1	A	109	ASN	N-CA	6.37	1.55	1.46
1	C	44	ASP	CG-OD2	-6.35	1.13	1.25
1	C	47	MET	C-O	6.35	1.31	1.23
1	A	66	LYS	CA-C	6.32	1.61	1.52
1	C	75	TYR	CZ-OH	6.32	1.51	1.38
1	A	35	GLN	CA-C	6.31	1.61	1.52
1	C	65	GLY	N-CA	6.31	1.55	1.45
1	C	66	LYS	C-N	-6.30	1.25	1.33
1	B	72	ASN	C-O	6.29	1.32	1.24
1	A	109	ASN	CA-CB	-6.28	1.44	1.53
1	A	35	GLN	C-O	-6.27	1.16	1.24
1	C	23	THR	N-CA	6.27	1.53	1.46
1	A	101	MET	CA-CB	6.26	1.62	1.53
1	C	31	GLY	N-CA	-6.26	1.35	1.45
1	B	71	GLN	N-CA	6.25	1.53	1.46
1	A	69	GLY	C-O	6.22	1.32	1.23
1	C	54	ASP	C-O	6.22	1.31	1.23
1	A	21	GLU	C-N	6.21	1.42	1.33
1	A	39	VAL	CA-C	-6.19	1.45	1.52
1	C	92	ASP	CG-OD2	6.18	1.37	1.25
1	A	77	LYS	CA-CB	6.18	1.62	1.53
1	C	5	VAL	CA-CB	6.16	1.62	1.54
1	A	54	ASP	CA-C	6.15	1.61	1.53
1	B	81	GLY	N-CA	6.13	1.53	1.45
1	C	63	SER	C-O	-6.13	1.16	1.23
1	B	32	LYS	C-N	-6.11	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	PHE	CB-CG	6.08	1.64	1.50
1	C	73	ARG	CA-C	-6.08	1.44	1.52
1	A	29	ALA	CA-CB	6.08	1.62	1.53
1	B	40	HIS	CG-CD2	6.08	1.42	1.35
1	A	74	ASN	CG-ND2	6.04	1.46	1.33
1	B	112	THR	CA-C	6.03	1.60	1.52
1	C	66	LYS	CE-NZ	6.01	1.67	1.49
1	C	22	LEU	C-N	-5.98	1.26	1.33
1	B	39	VAL	CA-C	5.98	1.59	1.52
1	A	69	GLY	N-CA	-5.96	1.36	1.45
1	A	28	GLN	CG-CD	-5.95	1.37	1.52
1	B	44	ASP	CB-CG	5.94	1.67	1.52
1	B	85	ASP	N-CA	5.94	1.53	1.46
1	B	69	GLY	C-N	5.94	1.42	1.33
1	A	114	ALA	N-CA	5.93	1.57	1.46
1	A	71	GLN	N-CA	5.92	1.53	1.46
1	B	36	TYR	CD2-CE2	5.92	1.56	1.38
1	C	28	GLN	C-N	5.92	1.42	1.33
1	B	37	ILE	CA-CB	-5.92	1.47	1.54
1	B	41	VAL	CA-C	5.91	1.59	1.52
1	B	96	ILE	C-O	5.90	1.30	1.24
1	C	40	HIS	CE1-NE2	5.89	1.38	1.32
1	C	27	ALA	N-CA	5.87	1.53	1.46
1	B	88	HIS	C-O	-5.85	1.16	1.23
1	B	31	GLY	C-O	5.85	1.32	1.24
1	C	74	ASN	CA-C	-5.83	1.45	1.52
1	C	91	PRO	C-O	5.82	1.31	1.24
1	B	22	LEU	C-O	5.82	1.31	1.24
1	A	15	PRO	C-O	5.81	1.30	1.23
1	A	22	LEU	CA-C	5.80	1.60	1.52
1	B	85	ASP	C-N	-5.80	1.25	1.33
1	C	11	ARG	C-O	-5.80	1.17	1.24
1	A	64	ILE	CA-CB	5.75	1.59	1.53
1	B	43	PRO	CA-C	5.74	1.60	1.52
1	A	40	HIS	CE1-NE2	5.72	1.38	1.32
1	A	31	GLY	C-O	5.72	1.31	1.24
1	B	15	PRO	C-O	5.67	1.30	1.23
1	B	25	GLN	C-O	5.67	1.30	1.24
1	A	42	VAL	CA-C	-5.65	1.47	1.52
1	C	79	LEU	CA-C	5.63	1.60	1.52
1	A	93	ARG	CZ-NH1	5.62	1.40	1.32
1	C	69	GLY	CA-C	5.62	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	25	GLN	CA-CB	5.62	1.63	1.53
1	A	6	ASN	CA-C	-5.62	1.46	1.52
1	B	2	MET	CG-SD	5.59	1.94	1.80
1	A	91	PRO	CA-C	-5.59	1.43	1.52
1	B	69	GLY	C-O	-5.59	1.17	1.23
1	B	65	GLY	C-O	5.57	1.32	1.23
1	A	92	ASP	CG-OD2	5.57	1.35	1.25
1	C	15	PRO	N-CD	-5.56	1.40	1.47
1	B	99	TYR	CA-C	5.56	1.59	1.52
1	C	82	LEU	CA-C	-5.55	1.45	1.52
1	C	37	ILE	CA-C	-5.54	1.46	1.52
1	C	98	TYR	CA-C	5.54	1.59	1.52
1	A	1	PRO	N-CA	5.54	1.55	1.47
1	A	29	ALA	CA-C	-5.54	1.45	1.52
1	A	28	GLN	N-CA	5.53	1.53	1.46
1	A	18	PHE	CA-CB	5.52	1.61	1.53
1	B	46	LEU	C-N	-5.50	1.26	1.33
1	A	5	VAL	C-O	5.50	1.30	1.24
1	A	96	ILE	CA-C	-5.49	1.45	1.52
1	C	1	PRO	CA-CB	-5.49	1.42	1.53
1	A	68	GLY	C-N	5.49	1.41	1.33
1	B	62	HIS	C-N	5.48	1.40	1.33
1	A	110	GLY	C-O	5.48	1.31	1.24
1	B	18	PHE	C-N	-5.48	1.26	1.34
1	A	84	SER	N-CA	5.47	1.52	1.46
1	C	31	GLY	C-N	5.45	1.44	1.33
1	C	26	LEU	CB-CG	5.44	1.64	1.53
1	B	93	ARG	C-O	5.43	1.31	1.23
1	C	27	ALA	CA-C	5.43	1.59	1.52
1	C	47	MET	CB-CG	-5.42	1.36	1.52
1	B	114	ALA	CA-CB	-5.42	1.34	1.52
1	C	19	LEU	CB-CG	5.41	1.64	1.53
1	C	22	LEU	CB-CG	5.41	1.64	1.53
1	C	74	ASN	CG-ND2	-5.41	1.21	1.33
1	C	112	THR	C-O	5.39	1.30	1.23
1	A	44	ASP	C-N	5.39	1.41	1.33
1	C	28	GLN	CA-CB	5.39	1.61	1.53
1	B	93	ARG	CZ-NH1	5.39	1.40	1.32
1	A	100	ASP	C-N	5.37	1.41	1.33
1	B	9	VAL	C-N	5.37	1.40	1.33
1	C	107	GLY	CA-C	-5.37	1.45	1.52
1	A	111	SER	C-N	-5.36	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	ASN	CG-OD1	5.36	1.33	1.23
1	C	67	ILE	N-CA	-5.36	1.39	1.46
1	C	16	GLU	CB-CG	-5.34	1.36	1.52
1	B	77	LYS	CA-CB	5.33	1.61	1.53
1	C	25	GLN	CD-NE2	5.32	1.44	1.33
1	C	35	GLN	N-CA	5.32	1.52	1.46
1	B	47	MET	CG-SD	5.31	1.94	1.80
1	C	43	PRO	CA-C	-5.29	1.44	1.52
1	C	18	PHE	C-N	-5.29	1.26	1.34
1	C	66	LYS	CD-CE	5.28	1.68	1.52
1	C	12	ALA	N-CA	5.27	1.53	1.46
1	C	45	GLN	CA-CB	5.27	1.61	1.53
1	A	91	PRO	C-N	5.26	1.42	1.33
1	A	92	ASP	C-N	5.26	1.41	1.33
1	C	68	GLY	CA-C	-5.26	1.45	1.51
1	C	29	ALA	C-O	5.25	1.30	1.24
1	A	25	GLN	CA-CB	5.23	1.61	1.53
1	B	52	THR	C-N	-5.23	1.26	1.33
1	B	78	LEU	CA-CB	-5.23	1.45	1.53
1	C	21	GLU	C-O	-5.23	1.18	1.24
1	C	53	ASN	CA-CB	-5.23	1.45	1.53
1	B	52	THR	N-CA	5.22	1.52	1.45
1	C	28	GLN	CA-C	-5.22	1.46	1.52
1	A	19	LEU	N-CA	5.22	1.52	1.46
1	B	32	LYS	N-CA	-5.22	1.37	1.45
1	C	74	ASN	CG-OD1	5.21	1.33	1.23
1	B	78	LEU	CA-C	-5.21	1.46	1.52
1	A	107	GLY	CA-C	-5.20	1.47	1.52
1	C	34	ALA	N-CA	5.20	1.52	1.46
1	B	82	LEU	CB-CG	-5.20	1.43	1.53
1	B	61	LEU	C-O	5.19	1.29	1.24
1	A	37	ILE	CA-C	-5.19	1.46	1.52
1	B	26	LEU	CA-C	-5.17	1.46	1.52
1	C	55	PRO	C-N	5.17	1.40	1.33
1	C	75	TYR	CA-CB	5.15	1.61	1.53
1	C	25	GLN	CA-C	5.15	1.59	1.52
1	B	99	TYR	CE2-CZ	-5.15	1.25	1.38
1	C	67	ILE	C-N	5.14	1.38	1.33
1	A	63	SER	CA-C	-5.13	1.46	1.52
1	B	112	THR	C-N	-5.13	1.26	1.33
1	C	71	GLN	CB-CG	5.13	1.67	1.52
1	C	83	LEU	N-CA	5.13	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	LEU	CB-CG	5.12	1.63	1.53
1	B	10	PRO	N-CD	5.11	1.54	1.47
1	A	9	VAL	C-O	-5.11	1.18	1.24
1	A	99	TYR	CZ-OH	5.10	1.48	1.38
1	C	84	SER	N-CA	5.09	1.52	1.46
1	B	17	GLY	C-N	-5.07	1.27	1.33
1	C	94	VAL	N-CA	5.05	1.52	1.46
1	A	110	GLY	N-CA	5.03	1.52	1.45
1	C	11	ARG	N-CA	5.03	1.52	1.46
1	B	73	ARG	CA-CB	5.02	1.61	1.53

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	GLU	O-C-N	35.94	164.46	123.13
1	B	11	ARG	CD-NE-CZ	-27.92	85.31	124.40
1	C	16	GLU	CG-CD-OE1	-27.84	54.37	118.40
1	B	28	GLN	CG-CD-NE2	-26.73	76.30	116.40
1	C	11	ARG	NE-CZ-NH1	24.86	146.36	121.50
1	C	31	GLY	O-C-N	-24.05	91.26	122.28
1	B	11	ARG	NH1-CZ-NH2	-23.89	88.24	119.30
1	A	28	GLN	OE1-CD-NE2	-22.86	99.74	122.60
1	C	11	ARG	NE-CZ-NH2	-22.71	98.76	119.20
1	C	86	ARG	NE-CZ-NH1	22.66	144.16	121.50
1	C	36	TYR	CZ-CE2-CD2	-22.65	78.82	119.60
1	C	16	GLU	CA-CB-CG	-20.87	72.37	114.10
1	A	35	GLN	CG-CD-NE2	20.58	147.27	116.40
1	B	11	ARG	NE-CZ-NH1	20.36	141.86	121.50
1	C	36	TYR	CD1-CE1-CZ	-18.88	85.62	119.60
1	C	16	GLU	CG-CD-OE2	-18.75	75.29	118.40
1	A	14	VAL	CA-C-O	18.14	129.85	119.15
1	A	15	PRO	O-C-N	-17.96	100.96	123.06
1	C	36	TYR	CE1-CZ-CE2	17.63	155.57	120.30
1	C	30	THR	CA-C-O	-17.10	98.83	119.18
1	C	29	ALA	CA-C-O	-16.91	101.47	120.24
1	C	16	GLU	CA-C-N	-16.67	88.74	121.41
1	C	16	GLU	C-N-CA	-16.67	88.74	121.41
1	C	53	ASN	OD1-CG-ND2	-16.46	106.14	122.60
1	A	35	GLN	OE1-CD-NE2	-16.30	106.30	122.60
1	B	28	GLN	CG-CD-OE1	16.03	152.86	120.80
1	B	31	GLY	CA-C-O	15.98	136.76	119.02
1	C	16	GLU	CB-CG-CD	15.82	139.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	THR	N-CA-C	-15.52	94.34	113.28
1	A	16	GLU	CA-C-N	-15.00	100.56	122.46
1	A	16	GLU	C-N-CA	-15.00	100.56	122.46
1	B	36	TYR	CE1-CZ-CE2	14.56	149.43	120.30
1	A	73	ARG	CD-NE-CZ	-14.54	104.04	124.40
1	C	33	PRO	N-CA-CB	-14.45	88.08	103.25
1	C	36	TYR	CB-CG-CD2	-14.43	99.16	120.80
1	C	33	PRO	N-CD-CG	-14.30	81.74	103.20
1	B	28	GLN	OE1-CD-NE2	-14.20	108.40	122.60
1	C	22	LEU	CA-C-O	-14.19	105.38	120.42
1	B	31	GLY	O-C-N	-14.14	104.43	122.39
1	B	25	GLN	OE1-CD-NE2	-13.89	108.71	122.60
1	C	33	PRO	O-C-N	13.81	141.29	122.64
1	B	36	TYR	CZ-CE2-CD2	-13.54	95.23	119.60
1	A	25	GLN	OE1-CD-NE2	-13.44	109.16	122.60
1	B	77	LYS	CG-CD-CE	-13.34	80.62	111.30
1	B	2	MET	CG-SD-CE	-13.22	71.81	100.90
1	C	36	TYR	CE1-CZ-OH	-13.20	80.30	119.90
1	A	25	GLN	CG-CD-OE1	12.96	146.72	120.80
1	A	88	HIS	CG-CD2-NE2	-12.70	94.50	107.20
1	B	25	GLN	CG-CD-OE1	12.36	145.51	120.80
1	C	86	ARG	NH1-CZ-NH2	-12.36	103.24	119.30
1	C	35	GLN	CA-CB-CG	-12.32	89.45	114.10
1	C	81	GLY	O-C-N	-12.31	110.25	122.19
1	C	16	GLU	N-CA-CB	-12.21	89.67	110.17
1	C	27	ALA	CA-C-O	-12.18	106.72	120.24
1	C	33	PRO	CA-C-O	-12.18	98.44	120.60
1	C	32	LYS	CA-C-O	-12.18	109.96	120.19
1	B	25	GLN	CG-CD-NE2	-11.90	98.54	116.40
1	B	77	LYS	CD-CE-NZ	11.90	149.97	111.90
1	A	15	PRO	CA-C-O	11.88	136.16	121.67
1	C	22	LEU	O-C-N	11.88	135.69	122.15
1	C	31	GLY	CA-C-O	11.84	131.59	119.04
1	B	25	GLN	CB-CG-CD	-11.78	92.57	112.60
1	C	86	ARG	CD-NE-CZ	-11.65	108.09	124.40
1	A	16	GLU	CG-CD-OE1	-11.54	91.86	118.40
1	C	25	GLN	OE1-CD-NE2	-11.44	111.16	122.60
1	A	13	SER	CA-C-N	-11.37	114.40	122.59
1	A	13	SER	C-N-CA	-11.37	114.40	122.59
1	C	82	LEU	CA-C-O	11.20	132.58	120.82
1	B	109	ASN	OD1-CG-ND2	11.19	133.79	122.60
1	A	88	HIS	ND1-CG-CD2	11.07	117.17	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	GLN	N-CA-CB	-11.03	93.83	110.16
1	C	67	ILE	O-C-N	-10.94	111.38	123.20
1	B	27	ALA	N-CA-C	-10.84	99.25	111.82
1	C	18	PHE	CA-C-O	-10.75	107.95	120.10
1	C	15	PRO	CA-C-O	10.69	133.53	121.34
1	C	16	GLU	CB-CA-C	-10.65	92.43	110.22
1	C	36	TYR	N-CA-C	-10.60	99.88	112.92
1	A	16	GLU	OE1-CD-OE2	10.58	148.30	122.90
1	C	31	GLY	N-CA-C	-10.42	101.64	115.40
1	C	64	ILE	O-C-N	10.35	134.73	122.62
1	C	81	GLY	CA-C-N	10.31	133.85	120.44
1	C	81	GLY	C-N-CA	10.31	133.85	120.44
1	C	53	ASN	CB-CG-OD1	10.30	141.40	120.80
1	A	16	GLU	N-CA-CB	-10.09	94.60	109.83
1	C	15	PRO	CA-C-N	-9.93	108.90	122.30
1	C	15	PRO	C-N-CA	-9.93	108.90	122.30
1	B	85	ASP	CA-C-O	-9.92	109.91	120.42
1	C	18	PHE	CA-CB-CG	-9.81	103.99	113.80
1	A	25	GLN	CG-CD-NE2	-9.81	101.69	116.40
1	C	84	SER	CA-C-O	-9.78	110.63	120.70
1	C	82	LEU	O-C-N	-9.77	112.00	122.07
1	C	20	SER	O-C-N	-9.72	111.06	122.15
1	B	47	MET	CG-SD-CE	9.71	122.26	100.90
1	C	18	PHE	O-C-N	9.59	133.44	122.22
1	A	88	HIS	CE1-NE2-CD2	9.59	118.59	109.00
1	C	68	GLY	CA-C-O	9.54	131.49	121.75
1	B	2	MET	CA-CB-CG	9.44	132.97	114.10
1	A	16	GLU	O-C-N	9.42	134.46	122.87
1	A	21	GLU	OE1-CD-OE2	9.31	145.24	122.90
1	B	29	ALA	CA-C-O	-9.28	108.84	119.79
1	C	50	SER	N-CA-C	-9.23	100.43	112.24
1	B	25	GLN	CA-C-O	-9.23	110.00	120.24
1	A	70	ALA	O-C-N	9.20	132.63	122.15
1	A	88	HIS	ND1-CE1-NE2	-9.15	99.25	108.40
1	B	1	PRO	N-CA-CB	9.05	112.96	103.00
1	C	11	ARG	CD-NE-CZ	-9.05	111.73	124.40
1	C	12	ALA	O-C-N	-9.04	109.99	122.46
1	A	73	ARG	NH1-CZ-NH2	-9.03	107.56	119.30
1	A	88	HIS	CB-CG-CD2	-9.01	119.49	131.20
1	C	44	ASP	OD1-CG-OD2	8.99	144.47	122.90
1	C	25	GLN	O-C-N	8.97	134.45	122.43
1	A	12	ALA	O-C-N	-8.97	110.08	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	THR	CA-CB-CG2	8.88	125.59	110.50
1	A	74	ASN	CB-CG-ND2	8.83	129.65	116.40
1	C	33	PRO	CA-N-CD	8.83	124.36	112.00
1	C	18	PHE	CD1-CE1-CZ	-8.76	104.23	120.00
1	B	36	TYR	OH-CZ-CE2	-8.75	93.65	119.90
1	B	27	ALA	CA-C-O	-8.72	109.94	119.97
1	B	54	ASP	CA-C-O	-8.65	110.80	121.01
1	A	101	MET	O-C-N	8.64	133.19	123.16
1	A	35	GLN	CG-CD-OE1	-8.61	103.58	120.80
1	C	46	LEU	CA-C-O	-8.49	111.72	121.66
1	B	17	GLY	CA-C-O	-8.48	109.86	119.10
1	B	54	ASP	CB-CG-OD2	-8.45	98.97	118.40
1	C	33	PRO	CB-CA-C	8.45	125.50	111.56
1	C	36	TYR	CA-CB-CG	-8.34	98.88	113.90
1	A	110	GLY	CA-C-O	-8.33	109.77	119.02
1	B	84	SER	CA-C-O	-8.23	111.74	120.55
1	C	88	HIS	ND1-CG-CD2	8.23	114.33	106.10
1	A	70	ALA	CA-C-N	-8.15	109.36	120.28
1	A	70	ALA	C-N-CA	-8.15	109.36	120.28
1	C	53	ASN	CB-CG-ND2	-8.12	104.22	116.40
1	A	16	GLU	CA-CB-CG	-8.12	97.86	114.10
1	B	51	GLY	CA-C-O	-8.05	110.51	119.04
1	C	36	TYR	CB-CA-C	-7.98	97.08	110.56
1	C	27	ALA	N-CA-CB	-7.97	98.32	110.20
1	A	14	VAL	CA-C-N	7.95	127.88	119.85
1	A	14	VAL	C-N-CA	7.95	127.88	119.85
1	B	28	GLN	N-CA-C	-7.94	102.57	111.14
1	A	19	LEU	CA-C-O	7.91	128.93	120.55
1	B	109	ASN	CB-CG-ND2	-7.90	104.55	116.40
1	A	113	PHE	CD1-CG-CD2	-7.89	106.76	118.60
1	C	88	HIS	CG-CD2-NE2	-7.87	99.33	107.20
1	C	28	GLN	O-C-N	-7.87	113.18	122.15
1	A	9	VAL	CA-C-N	-7.85	112.62	120.31
1	A	9	VAL	C-N-CA	-7.85	112.62	120.31
1	C	65	GLY	O-C-N	-7.84	115.46	122.91
1	A	113	PHE	CG-CD2-CE2	7.84	134.02	120.70
1	C	17	GLY	CA-C-O	-7.83	106.94	120.57
1	C	66	LYS	CA-C-O	-7.83	111.11	120.81
1	C	35	GLN	N-CA-C	-7.80	102.86	111.36
1	C	34	ALA	O-C-N	-7.80	111.05	122.43
1	A	18	PHE	CA-CB-CG	-7.71	106.09	113.80
1	A	14	VAL	O-C-N	-7.70	114.88	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	GLN	O-C-N	-7.69	113.38	122.15
1	C	109	ASN	CA-CB-CG	-7.67	104.93	112.60
1	B	52	THR	O-C-N	-7.66	112.84	123.11
1	C	77	LYS	CG-CD-CE	-7.60	93.81	111.30
1	B	36	TYR	CD1-CE1-CZ	-7.59	105.93	119.60
1	A	51	GLY	CA-C-O	-7.57	110.61	119.02
1	A	19	LEU	O-C-N	-7.55	114.11	122.12
1	B	89	ILE	O-C-N	7.55	130.94	122.93
1	B	54	ASP	O-C-N	7.55	130.15	121.31
1	C	86	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	C	28	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	C	29	ALA	N-CA-CB	-7.46	99.09	110.20
1	A	68	GLY	CA-C-O	7.45	128.71	121.63
1	C	25	GLN	CA-C-N	-7.45	108.11	121.14
1	C	25	GLN	C-N-CA	-7.45	108.11	121.14
1	B	17	GLY	N-CA-C	-7.43	105.55	115.21
1	A	31	GLY	N-CA-C	-7.41	105.00	115.30
1	C	28	GLN	N-CA-C	-7.40	103.29	111.36
1	A	113	PHE	O-C-N	-7.39	113.47	122.34
1	A	11	ARG	CD-NE-CZ	-7.37	114.08	124.40
1	B	21	GLU	OE1-CD-OE2	-7.37	105.22	122.90
1	C	36	TYR	O-C-N	-7.35	113.52	122.34
1	B	28	GLN	CB-CG-CD	-7.29	100.21	112.60
1	C	32	LYS	CG-CD-CE	-7.29	94.54	111.30
1	B	29	ALA	O-C-N	-7.27	112.59	122.33
1	C	45	GLN	OE1-CD-NE2	-7.26	115.33	122.60
1	B	61	LEU	CA-C-O	-7.23	112.56	120.30
1	A	25	GLN	CB-CG-CD	-7.21	100.34	112.60
1	A	10	PRO	N-CA-CB	-7.21	95.09	103.23
1	B	18	PHE	CA-C-O	-7.20	112.79	120.42
1	A	28	GLN	N-CA-CB	-7.17	99.58	110.12
1	C	28	GLN	CA-CB-CG	-7.17	99.77	114.10
1	C	18	PHE	CE1-CZ-CE2	7.15	132.87	120.00
1	C	14	VAL	O-C-N	7.14	129.25	121.10
1	B	88	HIS	CA-C-O	7.09	129.76	121.54
1	C	88	HIS	CA-C-N	-7.09	112.77	122.91
1	C	88	HIS	C-N-CA	-7.09	112.77	122.91
1	C	109	ASN	CB-CG-OD1	-7.09	106.62	120.80
1	C	27	ALA	N-CA-C	-7.08	102.98	111.69
1	B	78	LEU	O-C-N	-7.07	114.45	122.09
1	A	29	ALA	CA-C-O	7.05	127.89	120.42
1	A	84	SER	CA-C-O	-7.01	113.48	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	C	100	ASP	CA-CB-CG	-6.96	105.64	112.60
1	C	77	LYS	CD-CE-NZ	-6.94	89.69	111.90
1	A	101	MET	CA-C-N	-6.94	111.50	121.42
1	A	101	MET	C-N-CA	-6.94	111.50	121.42
1	A	24	GLN	CG-CD-OE1	-6.92	106.95	120.80
1	A	24	GLN	OE1-CD-NE2	6.92	129.52	122.60
1	C	108	TRP	CD2-CE3-CZ3	-6.92	109.60	118.60
1	B	77	LYS	CA-C-O	-6.92	113.09	120.42
1	A	107	GLY	CA-C-O	6.91	127.26	121.18
1	A	93	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	A	109	ASN	CA-C-O	-6.89	112.30	120.57
1	A	14	VAL	N-CA-C	-6.88	100.81	107.76
1	C	68	GLY	N-CA-C	-6.85	100.74	110.75
1	C	79	LEU	CA-C-O	-6.83	111.73	119.79
1	B	82	LEU	CA-C-O	-6.80	113.21	120.42
1	B	85	ASP	OD1-CG-OD2	6.79	139.19	122.90
1	A	22	LEU	CA-C-O	-6.77	113.38	120.55
1	C	68	GLY	O-C-N	-6.76	117.05	123.81
1	B	73	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	B	84	SER	N-CA-C	-6.74	103.18	111.40
1	B	24	GLN	CA-C-O	-6.73	111.84	119.79
1	C	82	LEU	N-CA-CB	6.72	119.76	110.01
1	A	26	LEU	CA-C-N	-6.72	111.28	120.28
1	A	26	LEU	C-N-CA	-6.72	111.28	120.28
1	C	85	ASP	O-C-N	-6.72	114.49	122.15
1	B	30	THR	N-CA-C	-6.69	104.93	113.23
1	A	35	GLN	N-CA-CB	-6.68	98.97	110.32
1	C	20	SER	CA-C-O	6.68	127.50	120.42
1	C	9	VAL	O-C-N	-6.67	113.50	121.10
1	A	114	ALA	N-CA-CB	-6.67	100.39	110.40
1	C	50	SER	CA-C-O	-6.66	112.55	120.81
1	C	8	ASN	CA-C-O	-6.64	111.25	119.28
1	B	86	ARG	NE-CZ-NH1	6.63	128.13	121.50
1	B	53	ASN	OD1-CG-ND2	6.61	129.21	122.60
1	A	20	SER	O-C-N	-6.59	114.17	122.27
1	A	111	SER	CA-CB-OG	-6.59	97.93	111.10
1	C	1	PRO	N-CA-CB	6.57	110.23	103.00
1	C	22	LEU	CA-C-N	-6.55	111.93	120.44
1	C	22	LEU	C-N-CA	-6.55	111.93	120.44
1	C	34	ALA	N-CA-CB	-6.53	99.44	110.41
1	C	12	ALA	N-CA-C	-6.50	105.21	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	GLU	N-CA-C	6.49	118.36	111.28
1	A	88	HIS	CA-CB-CG	-6.48	107.32	113.80
1	B	53	ASN	CB-CG-ND2	-6.48	106.68	116.40
1	C	15	PRO	N-CA-CB	-6.44	97.58	103.31
1	B	114	ALA	N-CA-C	-6.43	92.99	111.00
1	C	30	THR	O-C-N	6.41	131.51	122.41
1	C	21	GLU	CA-C-N	-6.39	111.22	120.29
1	C	21	GLU	C-N-CA	-6.39	111.22	120.29
1	C	25	GLN	CG-CD-OE1	6.38	133.57	120.80
1	C	28	GLN	CA-C-O	-6.36	113.68	120.42
1	C	32	LYS	N-CA-C	6.35	118.07	110.07
1	C	25	GLN	CB-CG-CD	-6.34	101.82	112.60
1	B	102	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	C	72	ASN	CA-C-O	-6.33	113.71	120.42
1	C	35	GLN	CB-CG-CD	-6.33	101.85	112.60
1	A	70	ALA	N-CA-CB	-6.29	100.84	110.16
1	C	72	ASN	O-C-N	6.27	129.30	122.15
1	C	23	THR	N-CA-CB	-6.27	100.92	110.01
1	A	70	ALA	CA-C-O	-6.26	113.78	120.42
1	B	32	LYS	CA-C-N	6.25	126.21	120.03
1	B	32	LYS	C-N-CA	6.25	126.21	120.03
1	B	77	LYS	N-CA-CB	-6.25	100.92	110.16
1	B	102	ASN	CB-CG-OD1	6.24	133.29	120.80
1	A	33	PRO	CA-N-CD	6.24	120.73	112.00
1	C	44	ASP	CB-CG-OD2	-6.23	104.07	118.40
1	B	52	THR	CB-CA-C	-6.21	97.61	109.66
1	C	18	PHE	N-CA-CB	-6.17	100.72	110.22
1	C	36	TYR	CG-CD2-CE2	6.17	130.45	121.20
1	A	111	SER	CB-CA-C	-6.17	98.58	113.19
1	C	105	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	C	35	GLN	CA-C-O	-6.12	113.94	120.42
1	C	33	PRO	CA-C-N	-6.10	109.68	121.58
1	C	33	PRO	C-N-CA	-6.10	109.68	121.58
1	A	73	ARG	CB-CG-CD	-6.09	97.28	111.30
1	B	77	LYS	CA-CB-CG	-6.09	101.92	114.10
1	B	88	HIS	CA-CB-CG	-6.07	107.73	113.80
1	C	111	SER	N-CA-CB	-6.07	100.71	110.55
1	C	9	VAL	N-CA-CB	-6.07	102.71	111.21
1	A	86	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	C	46	LEU	CB-CA-C	6.05	121.40	111.41
1	B	18	PHE	N-CA-C	-6.05	104.76	111.36
1	C	44	ASP	CA-C-N	-6.05	111.73	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ASP	C-N-CA	-6.05	111.73	122.07
1	B	52	THR	CA-CB-OG1	6.04	118.66	109.60
1	B	35	GLN	CG-CD-NE2	6.04	125.46	116.40
1	B	25	GLN	N-CA-C	-6.02	104.29	111.69
1	A	66	LYS	N-CA-C	-6.02	105.89	113.23
1	B	74	ASN	CB-CG-OD1	-6.00	108.80	120.80
1	C	24	GLN	CB-CG-CD	-6.00	102.40	112.60
1	A	14	VAL	CB-CA-C	-6.00	104.30	110.71
1	A	28	GLN	CG-CD-NE2	5.99	125.38	116.40
1	C	32	LYS	CA-CB-CG	-5.99	102.12	114.10
1	B	10	PRO	N-CD-CG	-5.99	94.22	103.20
1	B	44	ASP	OD1-CG-OD2	5.98	137.26	122.90
1	A	2	MET	CG-SD-CE	-5.98	87.74	100.90
1	C	9	VAL	CA-C-O	5.98	127.97	119.95
1	B	29	ALA	CA-C-N	5.98	132.18	121.66
1	B	29	ALA	C-N-CA	5.98	132.18	121.66
1	A	86	ARG	NH1-CZ-NH2	-5.97	111.53	119.30
1	C	83	LEU	CA-C-O	-5.97	113.10	119.97
1	A	54	ASP	CA-CB-CG	-5.94	106.66	112.60
1	A	21	GLU	CG-CD-OE2	-5.93	104.77	118.40
1	A	108	TRP	CA-C-N	-5.92	114.21	122.74
1	A	108	TRP	C-N-CA	-5.92	114.21	122.74
1	C	73	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	66	LYS	CA-C-O	-5.92	113.31	120.12
1	B	73	ARG	CA-C-O	-5.92	113.17	119.97
1	B	105	ASN	OD1-CG-ND2	5.91	128.51	122.60
1	B	9	VAL	CA-C-O	5.91	124.94	119.62
1	A	29	ALA	N-CA-C	5.90	117.80	111.36
1	C	28	GLN	N-CA-CB	-5.90	101.43	110.16
1	A	96	ILE	O-C-N	-5.88	117.06	123.18
1	C	74	ASN	CA-C-O	5.88	126.65	120.42
1	B	74	ASN	CB-CG-ND2	5.86	125.19	116.40
1	B	52	THR	CA-C-O	-5.86	114.61	121.46
1	B	88	HIS	N-CA-C	5.85	119.50	111.54
1	B	96	ILE	CA-C-O	-5.85	114.31	120.39
1	C	101	MET	O-C-N	5.84	129.90	123.01
1	C	99	TYR	CD1-CE1-CZ	-5.82	109.12	119.60
1	B	27	ALA	O-C-N	-5.81	115.12	122.27
1	C	18	PHE	CA-C-N	-5.79	111.51	120.31
1	C	18	PHE	C-N-CA	-5.79	111.51	120.31
1	C	92	ASP	CB-CG-OD2	-5.79	105.08	118.40
1	C	65	GLY	CA-C-N	5.78	130.78	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	GLY	C-N-CA	5.78	130.78	122.40
1	C	80	CYS	N-CA-C	-5.77	105.07	111.71
1	C	85	ASP	N-CA-CB	-5.76	101.63	110.16
1	B	27	ALA	CA-C-N	5.76	128.28	120.44
1	B	27	ALA	C-N-CA	5.76	128.28	120.44
1	C	66	LYS	N-CA-C	-5.76	104.86	112.24
1	B	28	GLN	O-C-N	-5.75	115.88	122.09
1	B	69	GLY	N-CA-C	5.74	119.16	112.50
1	C	67	ILE	CA-CB-CG1	-5.71	100.69	110.40
1	A	18	PHE	CD1-CG-CD2	5.69	127.13	118.60
1	A	113	PHE	CB-CG-CD2	5.69	130.37	120.70
1	A	111	SER	CA-C-O	-5.68	114.62	121.32
1	B	21	GLU	N-CA-C	-5.67	105.10	111.28
1	C	17	GLY	O-C-N	5.63	130.02	122.70
1	C	21	GLU	O-C-N	5.61	128.07	122.12
1	B	69	GLY	CA-C-O	5.61	127.06	121.00
1	A	33	PRO	N-CD-CG	-5.60	94.80	103.20
1	C	109	ASN	OD1-CG-ND2	5.60	128.20	122.60
1	B	92	ASP	CB-CG-OD1	5.60	131.28	118.40
1	C	27	ALA	O-C-N	5.59	129.49	122.23
1	B	99	TYR	CE1-CZ-CE2	5.58	131.47	120.30
1	A	15	PRO	CA-N-CD	-5.58	104.19	112.00
1	C	36	TYR	N-CA-CB	-5.58	102.42	110.56
1	B	52	THR	N-CA-C	5.57	118.65	109.85
1	C	74	ASN	CB-CG-OD1	-5.56	109.67	120.80
1	A	27	ALA	N-CA-CB	-5.55	101.97	110.12
1	A	11	ARG	O-C-N	5.53	127.98	122.12
1	C	16	GLU	N-CA-C	-5.52	100.18	108.96
1	B	6	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	C	32	LYS	CA-C-N	-5.50	112.96	119.84
1	C	32	LYS	C-N-CA	-5.50	112.96	119.84
1	B	50	SER	O-C-N	-5.48	112.73	122.21
1	B	19	LEU	O-C-N	-5.47	115.54	122.27
1	A	93	ARG	NH1-CZ-NH2	-5.46	112.20	119.30
1	C	108	TRP	CE2-CD2-CE3	5.44	124.24	118.80
1	C	51	GLY	N-CA-C	-5.43	107.75	115.30
1	B	86	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	B	35	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	B	100	ASP	CA-CB-CG	-5.42	107.18	112.60
1	B	113	PHE	O-C-N	-5.41	114.54	122.43
1	B	88	HIS	ND1-CE1-NE2	-5.40	103.00	108.40
1	B	22	LEU	O-C-N	-5.40	116.00	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	SER	N-CA-C	-5.40	105.33	112.24
1	C	81	GLY	N-CA-C	-5.40	105.86	112.77
1	C	79	LEU	O-C-N	5.38	129.54	122.33
1	B	49	PHE	CD1-CG-CD2	5.38	126.67	118.60
1	C	73	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	A	47	MET	O-C-N	-5.34	116.70	123.17
1	B	93	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
1	C	70	ALA	CA-C-N	-5.34	112.19	120.31
1	C	70	ALA	C-N-CA	-5.34	112.19	120.31
1	C	26	LEU	N-CA-C	-5.33	106.28	112.89
1	A	68	GLY	O-C-N	-5.33	117.43	123.61
1	B	71	GLN	N-CA-C	-5.33	105.37	111.07
1	B	108	TRP	CG-CD2-CE3	-5.33	128.57	133.90
1	C	10	PRO	N-CA-CB	-5.32	97.22	103.23
1	B	110	GLY	O-C-N	5.32	129.10	122.34
1	A	75	TYR	CG-CD1-CE1	-5.31	113.23	121.20
1	C	92	ASP	CA-C-O	-5.31	112.17	119.12
1	C	99	TYR	CE1-CZ-CE2	5.30	130.91	120.30
1	B	88	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	B	12	ALA	O-C-N	-5.30	115.15	122.46
1	A	77	LYS	CG-CD-CE	-5.29	99.12	111.30
1	C	12	ALA	CA-C-N	5.28	131.87	121.58
1	C	12	ALA	C-N-CA	5.28	131.87	121.58
1	B	24	GLN	CA-CB-CG	-5.26	103.57	114.10
1	B	81	GLY	CA-C-O	-5.26	115.09	120.66
1	C	11	ARG	CA-C-N	-5.25	110.80	121.18
1	C	11	ARG	C-N-CA	-5.25	110.80	121.18
1	C	9	VAL	CA-CB-CG2	-5.24	101.49	110.40
1	B	82	LEU	N-CA-C	-5.22	105.67	111.36
1	C	78	LEU	N-CA-C	5.20	116.95	111.28
1	B	88	HIS	CA-C-N	-5.18	115.50	122.91
1	B	88	HIS	C-N-CA	-5.18	115.50	122.91
1	C	109	ASN	CB-CG-ND2	5.17	124.16	116.40
1	B	22	LEU	CA-C-N	5.15	127.13	120.44
1	B	22	LEU	C-N-CA	5.15	127.13	120.44
1	C	4	ILE	CB-CG1-CD1	-5.14	103.00	113.80
1	B	49	PHE	O-C-N	5.13	129.62	123.36
1	B	11	ARG	CA-C-O	5.13	126.17	120.63
1	A	21	GLU	O-C-N	-5.13	116.31	122.15
1	A	9	VAL	CA-CB-CG2	-5.13	101.69	110.40
1	B	73	ARG	CA-CB-CG	-5.12	103.86	114.10
1	B	4	ILE	CB-CG1-CD1	-5.11	103.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PRO	N-CD-CG	5.10	110.86	103.20
1	A	109	ASN	CB-CG-OD1	-5.10	110.59	120.80
1	C	33	PRO	N-CA-C	5.10	122.97	112.47
1	B	93	ARG	N-CA-C	-5.10	104.68	111.87
1	B	20	SER	N-CA-C	-5.09	105.81	111.36
1	B	40	HIS	CG-CD2-NE2	-5.09	102.11	107.20
1	B	78	LEU	N-CA-C	-5.09	105.64	111.14
1	B	49	PHE	CE1-CZ-CE2	5.05	129.10	120.00
1	C	63	SER	CA-C-O	5.05	126.65	120.99
1	A	16	GLU	CB-CG-CD	-5.05	104.01	112.60
1	B	77	LYS	CB-CG-CD	-5.05	99.69	111.30
1	C	72	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	C	73	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	C	74	ASN	O-C-N	-5.04	116.41	122.15
1	C	88	HIS	O-C-N	5.04	129.16	122.41
1	B	114	ALA	CA-C-O	5.03	136.09	121.00
1	A	28	GLN	CB-CA-C	5.03	119.14	110.79
1	B	40	HIS	ND1-CG-CD2	5.02	111.12	106.10
1	B	108	TRP	CE2-CD2-CE3	5.02	123.82	118.80
1	C	77	LYS	N-CA-CB	-5.01	102.81	110.07
1	A	28	GLN	CG-CD-OE1	5.00	130.81	120.80
1	C	53	ASN	N-CA-CB	5.00	118.15	110.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLY	Mainchain
1	A	28	GLN	Sidechain
1	A	73	ARG	Sidechain
1	B	11	ARG	Sidechain
1	B	25	GLN	Sidechain
1	B	28	GLN	Sidechain
1	B	54	ASP	Sidechain
1	B	86	ARG	Sidechain,Mainchain
1	C	16	GLU	Sidechain
1	C	18	PHE	Sidechain
1	C	24	GLN	Sidechain
1	C	28	GLN	Sidechain
1	C	33	PRO	Mainchain
1	C	34	ALA	Mainchain
1	C	35	GLN	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	C	36	TYR	Sidechain
1	C	53	ASN	Sidechain

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	869	0	853	42	0
1	B	869	0	853	55	0
1	C	869	0	852	60	0
2	A	170	0	0	2	0
2	B	159	0	0	3	0
2	C	136	0	0	3	0
All	All	3072	0	2558	154	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 30.

All (154) 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:36:TYR:CB	1:C:36:TYR:CG	1.74	1.69
1:C:36:TYR:CE2	1:C:36:TYR:CZ	1.83	1.65
1:C:36:TYR:CD1	1:C:36:TYR:CE1	1.79	1.64
1:C:32:LYS:CA	1:C:32:LYS:CB	1.78	1.62
1:A:73:ARG:CD	1:A:73:ARG:CG	1.75	1.59
1:C:77:LYS:CD	1:C:77:LYS:CE	1.77	1.58
1:C:35:GLN:CA	1:C:35:GLN:CB	1.79	1.57
1:A:16:GLU:CA	1:A:16:GLU:CB	1.79	1.56
1:C:25:GLN:CB	1:C:25:GLN:CG	1.75	1.55
1:C:33:PRO:CD	1:C:33:PRO:CG	1.75	1.55
1:B:78:LEU:CG	1:B:78:LEU:CD1	1.80	1.54
1:C:17:GLY:CA	1:C:17:GLY:C	1.74	1.53
1:A:35:GLN:CD	1:A:35:GLN:CG	1.78	1.52
1:C:11:ARG:CD	1:C:11:ARG:NE	1.70	1.52
1:A:77:LYS:CE	1:A:77:LYS:NZ	1.72	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:CD	1:A:21:GLU:CG	1.79	1.51
1:B:11:ARG:CZ	1:B:11:ARG:NH1	1.67	1.51
1:A:16:GLU:CD	1:A:16:GLU:CG	1.83	1.51
1:A:17:GLY:N	1:A:17:GLY:CA	1.75	1.49
1:A:24:GLN:CD	1:A:24:GLN:CG	1.82	1.48
1:B:32:LYS:CD	1:B:32:LYS:CE	1.91	1.48
1:C:11:ARG:CZ	1:C:11:ARG:NH2	1.78	1.44
1:B:25:GLN:CB	1:B:25:GLN:CG	1.92	1.43
1:B:66:LYS:CD	1:B:66:LYS:CB	1.96	1.43
1:C:16:GLU:CA	1:C:16:GLU:HG2	1.49	1.42
1:C:36:TYR:CZ	1:C:36:TYR:OH	1.70	1.42
1:B:66:LYS:CD	1:B:66:LYS:CE	1.97	1.41
1:B:11:ARG:CD	1:B:11:ARG:NE	1.82	1.41
1:A:2:MET:CG	1:A:2:MET:SD	2.08	1.40
1:B:2:MET:SD	1:B:2:MET:CE	2.11	1.38
1:A:28:GLN:NE2	1:A:28:GLN:CD	1.84	1.33
1:B:25:GLN:NE2	1:B:25:GLN:CD	1.86	1.33
1:C:36:TYR:CZ	1:C:36:TYR:CD2	2.19	1.30
1:C:53:ASN:ND2	1:C:53:ASN:CG	1.88	1.30
1:C:32:LYS:CE	1:C:32:LYS:NZ	1.93	1.29
1:B:77:LYS:CE	1:B:77:LYS:NZ	1.97	1.28
1:A:28:GLN:CD	1:A:28:GLN:OE1	1.78	1.26
1:C:16:GLU:CA	1:C:16:GLU:C	2.15	1.19
1:C:16:GLU:CA	1:C:16:GLU:CB	2.20	1.19
1:C:16:GLU:CA	1:C:16:GLU:CG	2.20	1.18
1:B:66:LYS:CE	1:B:66:LYS:CG	2.23	1.16
1:C:36:TYR:CZ	1:C:36:TYR:CD1	2.37	1.12
1:C:88:HIS:CD2	1:C:88:HIS:NE2	1.69	1.11
1:C:36:TYR:CG	1:C:36:TYR:CZ	2.40	1.09
1:B:11:ARG:CZ	1:B:11:ARG:CD	2.31	1.08
1:C:16:GLU:CA	1:C:17:GLY:N	2.18	1.07
1:B:2:MET:CE	1:B:2:MET:CG	2.38	1.01
1:B:25:GLN:CB	1:B:25:GLN:CD	2.34	1.00
1:C:35:GLN:CA	1:C:35:GLN:CG	2.39	1.00
1:A:73:ARG:CD	1:A:73:ARG:CB	2.41	0.98
1:B:11:ARG:CZ	1:B:11:ARG:NH2	2.26	0.98
1:C:36:TYR:CG	1:C:36:TYR:CA	2.48	0.96
1:C:36:TYR:CE1	1:C:36:TYR:OH	2.19	0.95
1:C:36:TYR:CB	1:C:36:TYR:CD2	2.49	0.95
1:A:16:GLU:C	1:A:17:GLY:CA	2.40	0.94
1:C:77:LYS:CE	1:C:77:LYS:CG	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:HG2	1:C:16:GLU:OE1	1.72	0.90
1:A:2:MET:CG	1:A:2:MET:CE	2.51	0.88
1:A:16:GLU:CB	1:A:16:GLU:N	2.36	0.87
1:C:25:GLN:CB	1:C:25:GLN:CD	2.48	0.87
1:C:11:ARG:CD	1:C:11:ARG:CZ	2.53	0.87
1:C:53:ASN:ND2	1:C:53:ASN:CB	2.40	0.85
1:B:66:LYS:CD	1:B:66:LYS:HG3	1.33	0.85
1:B:66:LYS:CD	1:B:66:LYS:HG2	1.33	0.85
1:B:66:LYS:CG	1:B:66:LYS:HD3	1.33	0.84
1:B:25:GLN:CG	1:B:25:GLN:NE2	2.39	0.84
1:B:78:LEU:CD1	1:B:78:LEU:CD2	2.56	0.83
1:C:77:LYS:CD	1:C:77:LYS:NZ	2.40	0.83
1:A:16:GLU:CA	1:A:16:GLU:CG	2.56	0.82
1:B:66:LYS:CG	1:B:66:LYS:HD2	1.33	0.82
1:C:16:GLU:CG	1:C:16:GLU:CD	2.53	0.82
1:C:35:GLN:CB	1:C:35:GLN:N	2.43	0.81
1:B:2:MET:CE	1:B:2:MET:HG3	2.10	0.80
1:C:16:GLU:HG2	1:C:16:GLU:HA	1.62	0.78
1:C:62:HIS:HD2	2:C:176:HOH:O	1.67	0.78
1:A:73:ARG:CG	1:A:73:ARG:NE	2.47	0.77
1:B:66:LYS:HD3	1:B:66:LYS:CA	2.15	0.77
1:C:32:LYS:CA	1:C:32:LYS:CG	2.62	0.76
1:C:30:THR:O	1:C:66:LYS:HE2	1.88	0.74
1:B:58:LEU:HD13	1:C:2:MET:HE3	1.69	0.74
1:A:16:GLU:CB	1:A:16:GLU:C	2.62	0.71
1:B:25:GLN:HB3	1:B:78:LEU:HD21	1.71	0.71
1:C:32:LYS:CB	1:C:32:LYS:C	2.64	0.70
1:A:16:GLU:CG	1:A:16:GLU:OE1	2.39	0.70
1:B:32:LYS:CD	1:B:32:LYS:NZ	2.55	0.70
1:B:66:LYS:HD3	1:B:66:LYS:N	2.08	0.69
1:C:11:ARG:NE	1:C:11:ARG:NH2	2.39	0.69
1:C:16:GLU:CA	1:C:17:GLY:H	2.04	0.69
1:A:77:LYS:NZ	1:A:77:LYS:CD	2.55	0.68
1:A:2:MET:SD	1:A:2:MET:CB	2.79	0.68
1:B:66:LYS:CD	1:B:66:LYS:CA	2.68	0.68
1:B:11:ARG:CZ	1:B:11:ARG:HD3	2.23	0.68
1:A:21:GLU:CG	1:A:21:GLU:OE2	2.40	0.67
1:C:32:LYS:CB	1:C:32:LYS:N	2.56	0.67
1:C:16:GLU:CG	1:C:16:GLU:OE1	2.42	0.67
1:C:25:GLN:CG	1:C:25:GLN:CA	2.72	0.67
1:C:53:ASN:ND2	1:C:53:ASN:HB3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:CD	1:A:21:GLU:CB	2.67	0.66
2:B:203:HOH:O	1:C:2:MET:HE1	1.96	0.66
1:B:66:LYS:CE	1:B:66:LYS:HG2	2.23	0.66
1:A:2:MET:HE1	2:C:163:HOH:O	1.94	0.65
1:B:78:LEU:CD1	1:B:78:LEU:CB	2.69	0.65
1:B:2:MET:HG3	1:B:2:MET:HE2	1.78	0.64
1:C:35:GLN:CB	1:C:35:GLN:C	2.69	0.63
1:A:16:GLU:CB	1:A:16:GLU:CD	2.71	0.63
1:B:25:GLN:CG	1:B:78:LEU:HD11	2.29	0.63
1:B:66:LYS:CB	1:B:66:LYS:HD3	1.95	0.62
1:B:66:LYS:CD	1:B:66:LYS:CG	0.62	0.62
1:B:25:GLN:NE2	1:B:25:GLN:HG3	2.15	0.62
1:C:35:GLN:CA	1:C:35:GLN:HG2	2.28	0.61
1:C:16:GLU:CB	1:C:16:GLU:N	2.65	0.60
1:C:16:GLU:OE1	1:C:17:GLY:N	2.35	0.59
1:C:17:GLY:CA	1:C:17:GLY:O	2.44	0.58
1:B:66:LYS:HG3	1:B:66:LYS:NZ	2.19	0.58
1:A:34:ALA:HA	1:A:37:ILE:HD12	1.85	0.57
1:B:66:LYS:CE	1:B:66:LYS:HG3	2.27	0.57
1:A:16:GLU:CB	1:A:16:GLU:H	2.14	0.56
1:C:17:GLY:C	1:C:17:GLY:N	2.62	0.56
1:B:2:MET:CE	1:B:2:MET:CB	2.79	0.56
1:C:35:GLN:CB	1:C:35:GLN:H	2.20	0.54
1:B:66:LYS:CB	1:B:66:LYS:HD2	2.00	0.54
1:B:66:LYS:CG	1:B:66:LYS:NZ	2.70	0.54
1:C:16:GLU:CA	1:C:16:GLU:OE1	2.55	0.54
1:B:25:GLN:CD	1:B:25:GLN:CA	2.83	0.52
1:B:25:GLN:CG	1:B:25:GLN:CA	2.84	0.51
1:A:73:ARG:CB	1:A:73:ARG:HD2	2.35	0.51
1:A:35:GLN:HG3	2:A:191:HOH:O	2.10	0.51
1:A:35:GLN:CG	1:A:35:GLN:OE1	2.57	0.51
1:B:25:GLN:HG2	1:B:78:LEU:HD11	1.93	0.50
1:A:3:PHE:CE2	1:A:5:VAL:CG2	2.95	0.49
1:A:6:ASN:HD22	1:A:45:GLN:HG3	1.76	0.49
1:C:16:GLU:CG	1:C:16:GLU:OE2	2.61	0.48
1:B:2:MET:HE3	1:B:2:MET:HB2	1.96	0.47
1:B:47:MET:CE	1:B:58:LEU:HG	2.46	0.46
1:C:66:LYS:HE3	1:C:66:LYS:HB3	1.65	0.46
1:B:66:LYS:CD	1:B:66:LYS:NZ	2.70	0.45
1:A:109:ASN:HD22	1:C:91:PRO:HB2	1.81	0.45
1:A:73:ARG:CD	1:A:73:ARG:HB3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:CD2	2:C:176:HOH:O	2.53	0.45
1:B:4:ILE:HD11	2:B:211:HOH:O	2.17	0.45
1:B:2:MET:CE	1:B:2:MET:HB2	2.46	0.45
1:A:72:ASN:ND2	1:B:105:ASN:HD22	2.16	0.43
1:B:2:MET:CB	1:B:2:MET:HE3	2.47	0.43
1:A:69:GLY:HA2	2:B:137:HOH:O	2.18	0.43
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.59	0.43
1:B:47:MET:HE2	1:B:58:LEU:HG	2.01	0.42
1:A:6:ASN:ND2	2:A:126:HOH:O	2.52	0.42
1:B:53:ASN:OD1	1:B:53:ASN:C	2.62	0.42
1:A:16:GLU:O	1:A:17:GLY:CA	2.66	0.41
1:A:21:GLU:CG	1:A:21:GLU:OE1	2.54	0.41
1:A:16:GLU:C	1:A:17:GLY:HA3	2.41	0.41
1:B:27:ALA:HA	1:B:37:ILE:HD11	2.03	0.41
1:B:104:ALA:HA	1:B:114:ALA:HB2	2.02	0.40
1:A:2:MET:HE3	1:A:2:MET:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	112/114 (98%)	112 (100%)	0	0	100	100
1	B	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
1	C	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
All	All	336/342 (98%)	331 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	95/95 (100%)	94 (99%)	1 (1%)	65	38
1	B	95/95 (100%)	91 (96%)	4 (4%)	26	3
1	C	95/95 (100%)	93 (98%)	2 (2%)	47	14
All	All	285/285 (100%)	278 (98%)	7 (2%)	42	11

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	B	2	MET
1	B	25	GLN
1	B	47	MET
1	B	55	PRO
1	C	16	GLU
1	C	43	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	28	GLN
1	A	45	GLN
1	A	71	GLN
1	A	88	HIS
1	A	109	ASN
1	B	25	GLN
1	B	105	ASN
1	C	35	GLN
1	C	62	HIS
1	C	71	GLN
1	C	88	HIS
1	C	109	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	17:GLY	C	18:PHE	N	1.20
1	B	51:GLY	C	52:THR	N	1.19
1	C	33:PRO	C	34:ALA	N	1.16
1	C	30:THR	C	31:GLY	N	1.07

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	114/114 (100%)	-0.56	0 100 100	11, 17, 28, 39	0
1	B	114/114 (100%)	-0.50	0 100 100	12, 17, 31, 44	0
1	C	114/114 (100%)	-0.44	1 (0%) 81 84	13, 19, 38, 67	0
All	All	342/342 (100%)	-0.50	1 (0%) 90 92	11, 17, 33, 67	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	16	GLU	3.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.