



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:00 AM UTC

PDB ID : 4DFR / pdb_00004dfr
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI AND LACTO-BACILLUS CASEI DIHYDROFOLATE REDUCTASE REFINED AT 1.7 ANGSTROMS RESOLUTION. I. GENERAL FEATURES AND BINDING OF METHOTREXATE
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Deposited on : 1982-06-25
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

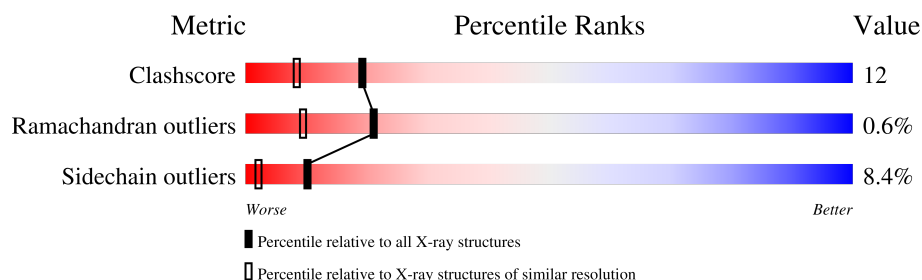
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	
1	B	159	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3035 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 DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	1	0
			1252	797	213	235	7			
1	B	159	Total	C	N	O	S	0	3	0
			1286	817	222	240	7			

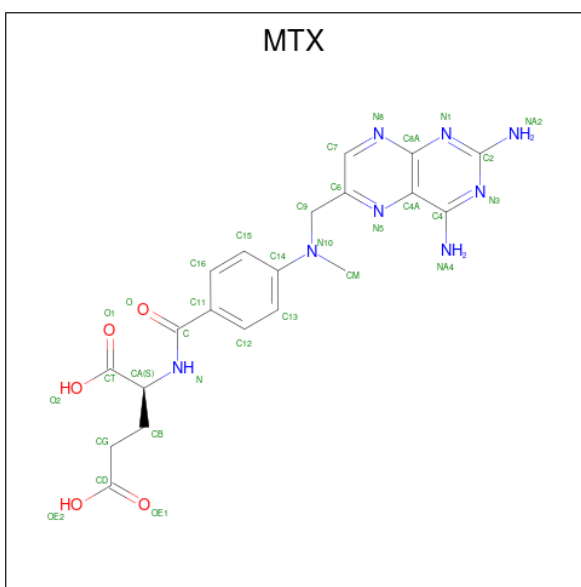
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	conflict	UNP P0ABQ4
A	154	LYS	GLU	conflict	UNP P0ABQ4
B	37	ASP	ASN	conflict	UNP P0ABQ4
B	154	LYS	GLU	conflict	UNP P0ABQ4

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is METHOTREXATE (CCD ID: MTX) (formula: C₂₀H₂₂N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 33	C 20	N 8	O 5	0	0
3	B	1	Total 33	C 20	N 8	O 5	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	239	Total O 239 239	0	0
5	B	189	Total O 189 189	0	0

3 Residue-property plots

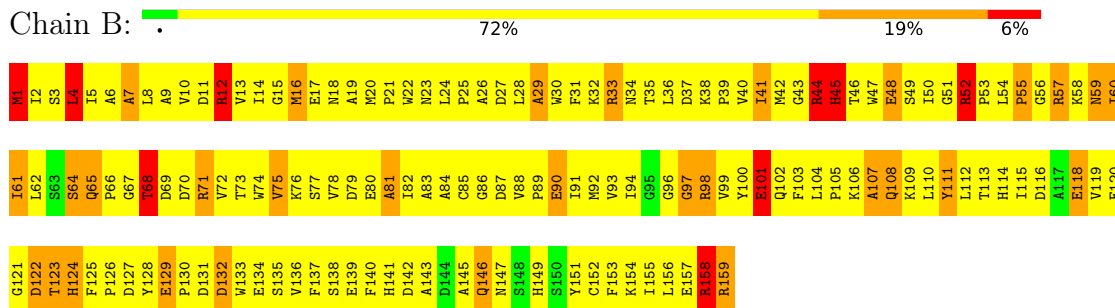
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: DIHYDROFOLATE REDUCTASE



- Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.22Å 93.22Å 73.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3035	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MTX, CL

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	4.25	268/1285 (20.9%)	4.65	434/1747 (24.8%)
1	B	4.25	279/1321 (21.1%)	4.98	451/1795 (25.1%)
All	All	4.25	547/2606 (21.0%)	4.82	885/3542 (25.0%)

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	7
1	B	0	15
All	All	0	22

All (547) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	PRO	C-O	18.84	1.47	1.23
1	A	43	GLY	C-O	18.49	1.40	1.23
1	A	109	LYS	C-N	-16.60	1.11	1.33
1	B	141	HIS	CD2-NE2	16.49	1.55	1.37
1	A	111	TYR	C-O	16.48	1.43	1.23
1	B	111	TYR	CA-C	-16.05	1.33	1.52
1	B	55	PRO	CA-C	-16.00	1.33	1.52
1	A	116	ASP	CA-C	-15.65	1.36	1.53
1	B	57	ARG	CZ-NH1	15.60	1.54	1.32
1	B	33	ARG	NE-CZ	15.45	1.50	1.33
1	A	103	PHE	CA-C	-15.02	1.32	1.52
1	B	93	VAL	C-O	14.85	1.42	1.24
1	A	152	CYS	CA-C	-14.78	1.34	1.52
1	A	115	ILE	CA-CB	14.65	1.73	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	LEU	C-N	-14.40	1.12	1.33
1	B	60	ILE	C-O	14.35	1.40	1.24
1	B	114	HIS	CG-ND1	14.08	1.53	1.38
1	A	111	TYR	C-N	-13.89	1.13	1.33
1	A	100	TYR	C-O	-13.51	1.08	1.24
1	B	138	SER	CB-OG	-13.31	1.15	1.42
1	B	93	VAL	CA-C	-13.16	1.36	1.52
1	B	20	MET	CA-C	-13.13	1.39	1.53
1	A	53	PRO	C-O	-13.13	1.09	1.23
1	B	44	ARG	CA-CB	12.79	1.73	1.53
1	B	102	GLN	CA-C	-12.78	1.36	1.52
1	A	33	ARG	CZ-NH2	12.75	1.50	1.33
1	B	114	HIS	C-N	-12.75	1.15	1.33
1	A	124	HIS	CE1-NE2	12.71	1.45	1.32
1	A	78	VAL	C-O	12.66	1.39	1.24
1	B	159	ARG	N-CA	12.59	1.70	1.46
1	A	143	ALA	C-N	-12.47	1.19	1.33
1	B	72	VAL	C-O	12.25	1.38	1.23
1	B	114	HIS	CG-CD2	-12.13	1.22	1.35
1	A	156	LEU	CA-C	-12.08	1.38	1.52
1	B	101	GLU	CA-CB	-11.95	1.34	1.53
1	A	93	VAL	C-O	11.88	1.37	1.24
1	B	59	ASN	C-N	-11.77	1.18	1.33
1	A	44	ARG	C-N	-11.67	1.17	1.34
1	A	123	THR	C-O	-11.61	1.09	1.23
1	A	17	GLU	CA-C	11.32	1.68	1.52
1	B	111	TYR	C-O	11.24	1.36	1.24
1	B	93	VAL	C-N	-11.19	1.20	1.33
1	B	57	ARG	CA-CB	10.94	1.74	1.54
1	B	149	HIS	CB-CG	10.90	1.65	1.50
1	B	116	ASP	C-O	10.82	1.37	1.23
1	A	151	TYR	CA-C	-10.79	1.38	1.52
1	B	124	HIS	C-O	10.78	1.37	1.23
1	A	30	TRP	C-N	-10.78	1.20	1.33
1	A	112	LEU	CA-C	-10.56	1.39	1.52
1	A	65	GLN	C-O	10.48	1.37	1.24
1	B	42	MET	C-O	-10.46	1.11	1.23
1	A	143	ALA	C-O	10.40	1.38	1.23
1	B	123	THR	CB-OG1	10.38	1.60	1.43
1	A	16	MET	CA-C	10.36	1.61	1.52
1	A	98	ARG	C-O	-10.33	1.12	1.24
1	B	2	ILE	CB-CG1	10.32	1.74	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ALA	C-O	10.28	1.37	1.23
1	B	111	TYR	N-CA	10.22	1.58	1.46
1	A	146	GLN	N-CA	10.19	1.59	1.46
1	A	131	ASP	C-O	10.18	1.37	1.24
1	B	59	ASN	CA-C	-10.18	1.40	1.52
1	B	59	ASN	C-O	10.17	1.36	1.24
1	B	159	ARG	NE-CZ	10.15	1.44	1.33
1	A	88	VAL	CA-CB	10.15	1.66	1.55
1	A	55	PRO	C-N	-10.14	1.20	1.33
1	A	74	TRP	CA-C	-10.14	1.40	1.52
1	A	113	THR	CB-OG1	-10.13	1.27	1.43
1	A	155	ILE	N-CA	-10.07	1.33	1.46
1	B	52	ARG	CA-C	-9.99	1.40	1.52
1	A	71	ARG	NE-CZ	-9.99	1.22	1.33
1	A	146	GLN	CA-C	-9.96	1.39	1.52
1	A	48	GLU	CA-C	-9.94	1.39	1.52
1	B	33	ARG	C-N	9.91	1.48	1.33
1	A	6	ALA	C-O	9.85	1.36	1.23
1	B	154	LYS	C-O	9.84	1.35	1.23
1	B	153	PHE	C-N	-9.79	1.18	1.33
1	A	124	HIS	CD2-NE2	-9.79	1.27	1.37
1	B	38	LYS	CA-C	9.69	1.62	1.52
1	B	44	ARG	NE-CZ	9.66	1.43	1.33
1	A	127	ASP	C-N	-9.61	1.19	1.33
1	A	151	TYR	C-N	-9.58	1.19	1.33
1	A	33	ARG	N-CA	9.58	1.58	1.46
1	A	11	ASP	CA-C	-9.54	1.38	1.52
1	A	133	TRP	NE1-CE2	9.51	1.48	1.37
1	B	133	TRP	C-N	-9.49	1.20	1.33
1	A	73	THR	C-O	-9.49	1.12	1.24
1	B	154	LYS	C-N	-9.48	1.20	1.33
1	A	13	VAL	CA-C	9.45	1.64	1.52
1	A	101	GLU	CA-C	-9.45	1.40	1.52
1	B	26	ALA	CA-C	-9.45	1.40	1.52
1	B	55	PRO	C-N	-9.42	1.21	1.33
1	A	44	ARG	CD-NE	9.41	1.59	1.46
1	B	1	MET	CA-C	9.39	1.72	1.52
1	B	151	TYR	C-N	-9.39	1.19	1.33
1	B	97	GLY	N-CA	9.36	1.58	1.45
1	A	126	PRO	N-CA	9.35	1.59	1.47
1	A	100	TYR	CA-C	9.35	1.65	1.52
1	B	100	TYR	CG-CD2	9.33	1.58	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	ALA	C-O	9.32	1.35	1.23
1	A	132	ASP	C-O	-9.27	1.11	1.24
1	A	5	ILE	C-N	-9.22	1.22	1.33
1	B	48	GLU	CA-C	-9.18	1.39	1.52
1	A	104	LEU	C-O	-9.16	1.15	1.24
1	B	43	GLY	C-N	9.14	1.45	1.33
1	B	62	LEU	C-N	9.11	1.45	1.33
1	A	133	TRP	CA-CB	9.05	1.71	1.53
1	A	72	VAL	C-N	-9.05	1.20	1.33
1	A	38	LYS	N-CA	-9.03	1.38	1.45
1	B	34	ASN	C-N	-9.03	1.20	1.33
1	B	3	SER	CA-C	-9.00	1.41	1.52
1	A	139	GLU	C-O	9.00	1.34	1.23
1	B	115	ILE	CA-C	8.97	1.63	1.52
1	B	131	ASP	CA-C	-8.95	1.40	1.52
1	A	41	ILE	C-O	-8.93	1.14	1.24
1	B	101	GLU	CA-C	-8.92	1.41	1.52
1	A	58	LYS	CA-C	8.86	1.64	1.52
1	A	146	GLN	CD-OE1	8.86	1.40	1.23
1	A	44	ARG	N-CA	-8.81	1.34	1.46
1	B	12	ARG	CZ-NH1	8.81	1.45	1.32
1	B	140	PHE	C-O	-8.79	1.13	1.23
1	A	90	GLU	CA-CB	-8.79	1.37	1.53
1	A	14	ILE	N-CA	-8.77	1.35	1.46
1	A	13	VAL	C-N	-8.76	1.23	1.33
1	A	93	VAL	CA-CB	8.74	1.64	1.54
1	A	25	PRO	CA-CB	-8.74	1.41	1.53
1	A	98	ARG	CD-NE	8.72	1.58	1.46
1	A	6	ALA	CA-CB	8.71	1.68	1.53
1	A	22	TRP	CD2-CE2	-8.70	1.26	1.41
1	A	48	GLU	CD-OE2	8.70	1.41	1.25
1	B	158	ARG	CA-CB	8.69	1.67	1.53
1	B	37	ASP	C-N	8.66	1.45	1.33
1	B	151	TYR	CA-C	-8.63	1.41	1.52
1	A	19	ALA	N-CA	8.61	1.56	1.46
1	A	57	ARG	CZ-NH2	8.59	1.44	1.33
1	A	159	ARG	C-O	8.59	1.40	1.23
1	B	54	LEU	CA-CB	8.58	1.69	1.53
1	B	42	MET	SD-CE	-8.54	1.58	1.79
1	A	52	ARG	CZ-NH1	8.51	1.44	1.32
1	A	149	HIS	CG-CD2	-8.50	1.26	1.35
1	A	144	ASP	CA-C	-8.49	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	ALA	C-O	8.42	1.34	1.24
1	A	24	LEU	CA-C	-8.41	1.42	1.52
1	B	72	VAL	CA-CB	8.39	1.67	1.54
1	A	51	GLY	N-CA	-8.37	1.33	1.45
1	B	20	MET	CA-CB	-8.36	1.41	1.53
1	A	29	ALA	CA-C	-8.35	1.42	1.52
1	A	85	CYS	N-CA	-8.34	1.35	1.46
1	B	152	CYS	C-N	-8.33	1.21	1.33
1	B	121	GLY	C-N	-8.33	1.22	1.33
1	B	74	TRP	CD1-NE1	-8.32	1.20	1.37
1	A	30	TRP	CA-C	-8.30	1.42	1.52
1	B	99	VAL	C-N	8.30	1.45	1.33
1	B	118	GLU	CD-OE2	8.29	1.41	1.25
1	B	138	SER	N-CA	8.28	1.55	1.46
1	B	12	ARG	NE-CZ	-8.27	1.24	1.33
1	B	68	THR	CB-OG1	8.27	1.56	1.43
1	B	104	LEU	N-CA	8.25	1.57	1.46
1	A	42	MET	CA-C	8.24	1.62	1.52
1	B	116	ASP	N-CA	8.22	1.57	1.46
1	A	124	HIS	ND1-CE1	-8.20	1.24	1.32
1	A	6	ALA	CA-C	-8.20	1.42	1.52
1	B	136	VAL	N-CA	-8.18	1.35	1.46
1	B	143	ALA	C-O	8.18	1.33	1.23
1	A	10	VAL	N-CA	8.17	1.56	1.46
1	B	33	ARG	C-O	-8.16	1.14	1.24
1	B	6	ALA	CA-CB	8.16	1.68	1.53
1	A	107	ALA	N-CA	-8.13	1.35	1.46
1	B	90	GLU	N-CA	8.11	1.55	1.46
1	B	131	ASP	CA-CB	8.11	1.67	1.53
1	A	109	LYS	C-O	-8.09	1.14	1.23
1	B	18	ASN	C-O	-8.09	1.11	1.23
1	A	89	PRO	C-N	8.08	1.44	1.33
1	B	115	ILE	C-O	-8.06	1.15	1.24
1	B	15	GLY	C-N	-8.04	1.22	1.33
1	B	5	ILE	CB-CG1	8.03	1.69	1.53
1	A	61	ILE	CA-C	8.01	1.62	1.52
1	B	81	ALA	N-CA	8.01	1.55	1.46
1	B	139	GLU	C-O	-7.98	1.14	1.23
1	A	33	ARG	CZ-NH1	7.98	1.44	1.32
1	B	74	TRP	C-N	7.97	1.44	1.33
1	A	127	ASP	CG-OD2	7.96	1.40	1.25
1	A	82	ILE	N-CA	-7.93	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	VAL	C-O	7.90	1.33	1.24
1	B	52	ARG	NE-CZ	7.90	1.41	1.33
1	A	152	CYS	C-O	7.89	1.33	1.24
1	A	1	MET	CA-CB	-7.84	1.37	1.53
1	A	120	GLU	N-CA	7.83	1.56	1.46
1	A	81	ALA	C-N	-7.80	1.24	1.33
1	B	91	ILE	CB-CG1	7.80	1.69	1.53
1	B	97	GLY	CA-C	-7.76	1.41	1.51
1	A	13	VAL	N-CA	7.74	1.56	1.46
1	B	7	ALA	C-N	-7.74	1.22	1.33
1	A	25	PRO	C-N	7.73	1.44	1.34
1	A	47	TRP	C-N	7.72	1.44	1.34
1	A	18	ASN	C-O	7.70	1.34	1.23
1	A	58	LYS	CD-CE	7.70	1.75	1.52
1	A	153	PHE	CA-C	-7.68	1.42	1.52
1	A	47	TRP	CD2-CE3	-7.67	1.27	1.40
1	B	143	ALA	N-CA	7.66	1.55	1.46
1	A	142	ASP	CA-C	7.65	1.62	1.52
1	A	121	GLY	C-N	7.64	1.45	1.33
1	A	20	MET	N-CA	7.63	1.56	1.45
1	B	8	LEU	CA-C	-7.60	1.43	1.52
1	B	76	LYS	CA-CB	7.59	1.65	1.53
1	A	144	ASP	C-O	7.59	1.32	1.23
1	B	57	ARG	NE-CZ	-7.57	1.24	1.33
1	A	9	ALA	C-N	-7.54	1.23	1.33
1	A	54	LEU	C-O	-7.53	1.14	1.24
1	B	159	ARG	CA-CB	-7.53	1.38	1.53
1	A	158	ARG	CD-NE	7.53	1.56	1.46
1	A	57	ARG	CD-NE	-7.52	1.35	1.46
1	B	61	ILE	C-O	7.49	1.32	1.24
1	A	43	GLY	N-CA	-7.49	1.37	1.45
1	A	111	TYR	CA-C	-7.48	1.43	1.53
1	B	36	LEU	C-N	-7.48	1.23	1.33
1	A	39	PRO	C-O	-7.46	1.15	1.23
1	B	114	HIS	CE1-NE2	-7.45	1.25	1.32
1	B	133	TRP	CA-C	7.44	1.61	1.52
1	B	17	GLU	CD-OE2	7.44	1.39	1.25
1	A	10	VAL	C-O	7.44	1.32	1.24
1	B	141	HIS	CE1-NE2	-7.42	1.25	1.32
1	B	85	CYS	C-O	7.42	1.33	1.24
1	B	24	LEU	C-O	-7.42	1.15	1.24
1	B	37	ASP	CA-CB	7.42	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	LEU	CA-CB	-7.37	1.45	1.53
1	A	9	ALA	CA-CB	-7.36	1.42	1.53
1	A	122	ASP	N-CA	7.35	1.55	1.46
1	A	116	ASP	N-CA	7.34	1.56	1.46
1	A	45	HIS	CA-C	7.34	1.62	1.52
1	A	135	SER	N-CA	-7.33	1.37	1.46
1	A	47	TRP	C-O	-7.33	1.15	1.24
1	B	38	LYS	CD-CE	7.33	1.74	1.52
1	B	18	ASN	CB-CG	7.32	1.70	1.52
1	B	32	LYS	C-N	-7.31	1.24	1.33
1	A	123	THR	CA-C	-7.29	1.43	1.52
1	A	105	PRO	N-CD	7.28	1.57	1.47
1	B	3	SER	C-O	7.27	1.32	1.23
1	A	60	ILE	CB-CG1	7.26	1.68	1.53
1	A	129	GLU	N-CA	7.24	1.56	1.46
1	B	23	ASN	CA-C	7.24	1.61	1.53
1	B	54	LEU	CA-C	7.24	1.61	1.52
1	B	120	GLU	CA-CB	7.23	1.63	1.53
1	B	78	VAL	C-O	-7.17	1.16	1.24
1	A	109	LYS	CB-CG	-7.16	1.30	1.52
1	A	82	ILE	CA-CB	-7.11	1.46	1.54
1	B	38	LYS	C-O	-7.10	1.14	1.24
1	B	89	PRO	C-O	7.10	1.32	1.24
1	A	122	ASP	CA-CB	7.09	1.64	1.53
1	A	49	SER	CA-C	7.09	1.61	1.52
1	B	44	ARG	C-O	-7.08	1.16	1.24
1	A	110	LEU	C-N	7.07	1.45	1.33
1	A	26	ALA	N-CA	-7.06	1.37	1.46
1	A	109	LYS	CE-NZ	7.06	1.70	1.49
1	A	56	GLY	N-CA	-7.05	1.35	1.45
1	B	42	MET	N-CA	-7.05	1.36	1.45
1	B	121	GLY	C-O	-7.05	1.15	1.24
1	A	101	GLU	N-CA	7.02	1.54	1.46
1	A	155	ILE	CA-CB	7.02	1.63	1.54
1	A	158	ARG	CA-C	7.02	1.61	1.52
1	B	35	THR	CA-CB	7.01	1.63	1.54
1	A	150	SER	CA-C	-7.01	1.44	1.52
1	A	95	GLY	C-N	-7.01	1.23	1.33
1	B	31	PHE	CA-C	7.00	1.61	1.52
1	B	111	TYR	CG-CD1	-7.00	1.24	1.39
1	A	88	VAL	C-O	-7.00	1.17	1.24
1	B	21	PRO	N-CD	7.00	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	ARG	CD-NE	6.95	1.55	1.46
1	A	92	MET	SD-CE	-6.92	1.62	1.79
1	B	157	GLU	C-O	-6.89	1.16	1.24
1	B	23	ASN	N-CA	-6.88	1.38	1.46
1	A	102	GLN	CD-OE1	6.88	1.36	1.23
1	B	48	GLU	N-CA	6.86	1.55	1.46
1	A	42	MET	C-N	6.85	1.42	1.33
1	A	104	LEU	C-N	-6.84	1.25	1.33
1	A	11	ASP	C-N	6.84	1.42	1.33
1	B	18	ASN	N-CA	6.84	1.55	1.46
1	A	9	ALA	N-CA	6.82	1.54	1.45
1	B	60	ILE	CA-C	-6.81	1.44	1.52
1	A	39	PRO	CA-C	6.78	1.60	1.52
1	B	106	LYS	CA-C	6.78	1.61	1.52
1	A	90	GLU	CA-C	6.77	1.60	1.52
1	A	26	ALA	CA-CB	6.76	1.64	1.53
1	B	30	TRP	C-N	-6.76	1.25	1.33
1	B	68	THR	C-O	6.74	1.32	1.23
1	B	33	ARG	CA-CB	6.72	1.63	1.53
1	B	147	ASN	CA-CB	6.72	1.63	1.53
1	A	16	MET	C-N	-6.71	1.24	1.33
1	B	141	HIS	CG-ND1	-6.70	1.30	1.38
1	B	4	LEU	C-O	6.69	1.32	1.24
1	B	70	ASP	CA-CB	6.68	1.64	1.53
1	A	65	GLN	CA-C	6.68	1.61	1.52
1	B	96	GLY	C-N	6.67	1.43	1.33
1	B	22	TRP	CZ3-CH2	-6.65	1.23	1.40
1	B	56	GLY	N-CA	-6.62	1.35	1.45
1	A	104	LEU	CB-CG	-6.61	1.40	1.53
1	A	53	PRO	CA-C	6.61	1.61	1.52
1	B	158	ARG	CA-C	6.60	1.61	1.52
1	B	133	TRP	N-CA	6.59	1.54	1.45
1	A	98	ARG	NE-CZ	6.59	1.40	1.33
1	B	51	GLY	CA-C	-6.58	1.42	1.51
1	B	50	ILE	CB-CG1	6.57	1.66	1.53
1	B	108	GLN	C-O	-6.56	1.15	1.24
1	B	98	ARG	CA-CB	6.56	1.64	1.53
1	B	39	PRO	N-CD	-6.56	1.38	1.47
1	B	107	ALA	C-N	-6.54	1.24	1.33
1	A	30	TRP	CD2-CE2	-6.54	1.30	1.41
1	B	87	ASP	C-N	-6.53	1.25	1.33
1	B	81	ALA	C-N	-6.53	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	TYR	N-CA	6.52	1.54	1.45
1	B	102	GLN	CD-OE1	6.51	1.35	1.23
1	B	72	VAL	C-N	-6.51	1.24	1.33
1	B	123	THR	C-N	-6.50	1.23	1.33
1	A	39	PRO	C-N	-6.49	1.25	1.33
1	A	47	TRP	CA-CB	-6.49	1.43	1.53
1	B	135	SER	CA-CB	6.49	1.62	1.53
1	A	108	GLN	CA-CB	-6.48	1.43	1.53
1	B	30	TRP	C-O	6.46	1.31	1.24
1	A	127	ASP	CA-CB	6.45	1.62	1.53
1	A	143	ALA	CA-CB	6.45	1.63	1.53
1	B	29	ALA	C-N	-6.45	1.25	1.33
1	B	125	PHE	CA-CB	6.44	1.63	1.53
1	B	6	ALA	CA-C	-6.43	1.44	1.52
1	B	18	ASN	CA-CB	-6.42	1.44	1.53
1	B	62	LEU	C-O	-6.41	1.16	1.24
1	A	142	ASP	C-O	-6.40	1.15	1.23
1	B	47	TRP	C-O	-6.40	1.16	1.24
1	A	38	LYS	CA-CB	-6.38	1.46	1.54
1	B	151	TYR	CZ-OH	-6.36	1.24	1.38
1	B	99	VAL	CA-CB	6.36	1.62	1.54
1	A	123	THR	CA-CB	6.35	1.62	1.53
1	A	41	ILE	N-CA	6.34	1.53	1.46
1	B	116	ASP	C-N	-6.34	1.24	1.33
1	A	107	ALA	CA-CB	6.34	1.63	1.53
1	A	34	ASN	N-CA	-6.33	1.37	1.46
1	B	71	ARG	NE-CZ	6.32	1.40	1.33
1	B	48	GLU	CD-OE2	6.32	1.37	1.25
1	B	72	VAL	CA-C	-6.31	1.45	1.52
1	B	114	HIS	ND1-CE1	-6.30	1.26	1.32
1	A	112	LEU	C-N	6.30	1.44	1.33
1	A	33	ARG	CA-CB	-6.30	1.43	1.53
1	B	52	ARG	CA-CB	6.29	1.63	1.53
1	A	63	SER	CA-C	6.29	1.60	1.52
1	A	48	GLU	CB-CG	-6.28	1.33	1.52
1	B	50	ILE	C-O	6.28	1.31	1.24
1	A	88	VAL	CA-C	-6.28	1.47	1.52
1	A	77	SER	CA-CB	6.25	1.65	1.53
1	A	62	LEU	CA-CB	-6.24	1.45	1.53
1	A	68	THR	C-O	6.24	1.31	1.24
1	B	110	LEU	N-CA	-6.23	1.38	1.46
1	A	106	LYS	CG-CD	6.23	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	ARG	CZ-NH2	6.22	1.41	1.33
1	A	120	GLU	CD-OE2	6.22	1.37	1.25
1	A	25	PRO	C-O	-6.22	1.16	1.24
1	B	50	ILE	C-N	-6.21	1.24	1.33
1	A	12	ARG	CZ-NH1	6.20	1.41	1.32
1	B	120	GLU	C-N	-6.19	1.27	1.33
1	B	153	PHE	CA-CB	-6.18	1.44	1.53
1	B	4	LEU	C-N	-6.18	1.25	1.33
1	A	22	TRP	CZ3-CH2	-6.16	1.25	1.40
1	B	20	MET	C-O	-6.16	1.16	1.24
1	A	137	PHE	C-N	-6.13	1.25	1.33
1	B	156	LEU	N-CA	6.11	1.53	1.46
1	B	88	VAL	C-N	6.11	1.41	1.34
1	A	141	HIS	CE1-NE2	6.09	1.38	1.32
1	A	34	ASN	C-O	6.07	1.32	1.24
1	A	149	HIS	ND1-CE1	-6.07	1.26	1.32
1	A	40	VAL	C-N	-6.06	1.25	1.33
1	B	98	ARG	CA-C	-6.04	1.44	1.52
1	B	16	MET	N-CA	6.04	1.53	1.45
1	A	129	GLU	CA-C	-6.03	1.45	1.52
1	B	108	GLN	C-N	6.03	1.41	1.33
1	A	85	CYS	CA-CB	6.02	1.63	1.53
1	B	101	GLU	CG-CD	6.02	1.67	1.52
1	B	19	ALA	CA-CB	-6.01	1.43	1.53
1	A	75	VAL	CA-CB	-6.01	1.45	1.55
1	A	92	MET	CA-C	-6.01	1.45	1.52
1	A	94	ILE	N-CA	6.00	1.53	1.46
1	B	28	LEU	N-CA	6.00	1.53	1.46
1	A	101	GLU	C-O	-6.00	1.17	1.24
1	B	127	ASP	N-CA	5.98	1.53	1.46
1	A	8	LEU	CA-C	-5.98	1.45	1.52
1	B	58	LYS	C-O	-5.95	1.16	1.24
1	B	14	ILE	CB-CG1	5.95	1.65	1.53
1	A	3	SER	C-O	-5.94	1.16	1.23
1	A	32	LYS	N-CA	5.94	1.53	1.46
1	B	57	ARG	CA-C	5.94	1.59	1.52
1	B	139	GLU	CD-OE2	5.93	1.36	1.25
1	B	88	VAL	N-CA	-5.92	1.39	1.46
1	A	141	HIS	CA-C	-5.92	1.45	1.52
1	B	122[A]	ASP	C-N	5.92	1.42	1.33
1	B	122[B]	ASP	C-N	5.92	1.42	1.33
1	A	142	ASP	C-N	-5.92	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	GLY	C-N	-5.92	1.25	1.33
1	B	129	GLU	CA-CB	5.92	1.62	1.53
1	B	26	ALA	C-N	5.92	1.41	1.33
1	B	43	GLY	C-O	5.91	1.32	1.23
1	A	124	HIS	CG-ND1	-5.91	1.31	1.38
1	B	149	HIS	C-N	-5.89	1.25	1.33
1	B	50	ILE	CA-C	5.88	1.60	1.52
1	B	112	LEU	C-O	-5.88	1.17	1.24
1	B	100	TYR	N-CA	5.87	1.53	1.46
1	B	77	SER	N-CA	-5.86	1.38	1.45
1	A	29	ALA	CA-CB	5.85	1.62	1.53
1	B	55	PRO	N-CA	5.85	1.54	1.47
1	B	107	ALA	N-CA	5.84	1.53	1.46
1	A	47	TRP	NE1-CE2	-5.83	1.31	1.37
1	B	74	TRP	NE1-CE2	5.83	1.43	1.37
1	B	43	GLY	CA-C	-5.81	1.39	1.52
1	A	85	CYS	C-O	5.81	1.31	1.24
1	A	78	VAL	CA-CB	-5.80	1.46	1.54
1	B	120	GLU	CA-C	-5.80	1.45	1.52
1	B	54	LEU	C-N	5.80	1.40	1.33
1	A	78	VAL	N-CA	-5.79	1.39	1.46
1	B	141	HIS	C-N	5.79	1.41	1.33
1	A	97	GLY	C-O	-5.79	1.16	1.23
1	A	52	ARG	CA-CB	5.78	1.62	1.53
1	B	78	VAL	C-N	5.77	1.41	1.34
1	B	54	LEU	C-O	-5.77	1.16	1.24
1	A	68	THR	CA-C	5.76	1.60	1.52
1	A	156	LEU	CB-CG	-5.76	1.42	1.53
1	B	74	TRP	CD2-CE2	-5.76	1.31	1.41
1	B	29	ALA	C-O	5.76	1.31	1.24
1	A	33	ARG	CD-NE	5.75	1.54	1.46
1	A	157	GLU	CA-CB	-5.75	1.44	1.53
1	B	17	GLU	C-N	5.74	1.41	1.33
1	B	89	PRO	CA-CB	5.74	1.61	1.53
1	A	12	ARG	CA-C	5.74	1.60	1.52
1	A	43	GLY	C-N	-5.73	1.25	1.33
1	A	44	ARG	CG-CD	-5.72	1.35	1.52
1	A	71	ARG	CD-NE	-5.72	1.38	1.46
1	B	31	PHE	C-O	-5.70	1.17	1.24
1	B	12	ARG	CZ-NH2	5.70	1.40	1.33
1	B	78	VAL	N-CA	-5.69	1.40	1.46
1	B	22	TRP	C-N	-5.69	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	CB-OG1	-5.68	1.34	1.43
1	A	110	LEU	C-O	-5.67	1.17	1.24
1	B	159	ARG	CA-C	5.66	1.64	1.52
1	A	135	SER	C-N	-5.65	1.25	1.33
1	B	46	THR	C-N	5.65	1.41	1.33
1	B	76	LYS	C-O	5.65	1.31	1.24
1	A	55	PRO	C-O	5.64	1.30	1.23
1	B	47	TRP	CE2-CZ2	5.64	1.51	1.39
1	A	30	TRP	CD2-CE3	5.63	1.49	1.40
1	A	158	ARG	CZ-NH2	5.62	1.40	1.33
1	B	90	GLU	C-O	5.62	1.30	1.23
1	A	98	ARG	CA-C	-5.61	1.45	1.52
1	B	116	ASP	CB-CG	5.61	1.66	1.52
1	A	110	LEU	CG-CD1	5.60	1.71	1.52
1	A	55	PRO	N-CA	-5.60	1.40	1.46
1	B	37	ASP	CG-OD1	5.59	1.35	1.25
1	B	109	LYS	CA-C	-5.59	1.45	1.52
1	B	17	GLU	CB-CG	-5.57	1.35	1.52
1	A	19	ALA	CA-C	-5.57	1.45	1.52
1	A	8	LEU	CB-CG	-5.56	1.42	1.53
1	B	104	LEU	C-O	5.56	1.31	1.24
1	B	59	ASN	CG-ND2	5.56	1.45	1.33
1	B	116	ASP	CG-OD1	5.56	1.35	1.25
1	B	11	ASP	C-N	5.55	1.41	1.33
1	B	139	GLU	CG-CD	-5.55	1.38	1.52
1	B	33	ARG	CG-CD	5.55	1.69	1.52
1	B	42	MET	CA-C	5.55	1.59	1.52
1	B	114	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	14	ILE	CB-CG1	5.53	1.64	1.53
1	A	7	ALA	C-N	5.52	1.40	1.33
1	A	131	ASP	C-N	-5.52	1.26	1.33
1	A	3	SER	CA-C	5.51	1.59	1.52
1	A	74	TRP	CA-CB	-5.51	1.46	1.53
1	B	59	ASN	CB-CG	-5.51	1.38	1.52
1	B	159	ARG	C-OXT	5.50	1.34	1.23
1	B	67	GLY	CA-C	-5.50	1.46	1.52
1	A	84	ALA	CA-CB	-5.49	1.43	1.53
1	A	41	ILE	CA-CB	5.48	1.60	1.54
1	A	70	ASP	CG-OD2	5.48	1.35	1.25
1	B	118	GLU	CD-OE1	5.48	1.35	1.25
1	A	112	LEU	C-O	-5.48	1.17	1.24
1	B	61	ILE	N-CA	5.48	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ARG	CZ-NH1	5.46	1.40	1.32
1	B	70	ASP	C-N	-5.46	1.25	1.33
1	A	1	MET	CA-C	5.45	1.64	1.52
1	B	157	GLU	CA-CB	-5.44	1.43	1.53
1	B	57	ARG	CZ-NH2	-5.43	1.26	1.33
1	A	30	TRP	NE1-CE2	-5.43	1.31	1.37
1	B	154	LYS	CD-CE	5.43	1.68	1.52
1	B	112	LEU	CB-CG	5.43	1.64	1.53
1	A	152	CYS	C-N	-5.42	1.25	1.33
1	B	100	TYR	CA-C	5.42	1.59	1.52
1	A	22	TRP	N-CA	-5.41	1.39	1.46
1	B	41	ILE	C-O	5.41	1.31	1.24
1	B	32	LYS	CA-C	-5.41	1.45	1.52
1	A	141	HIS	C-N	-5.41	1.26	1.33
1	B	11	ASP	C-O	-5.40	1.15	1.24
1	A	93	VAL	C-N	-5.39	1.27	1.33
1	A	51	GLY	C-N	-5.38	1.22	1.33
1	A	94	ILE	CA-C	-5.38	1.45	1.52
1	B	87	ASP	CA-C	5.37	1.60	1.53
1	A	141	HIS	CG-ND1	5.36	1.44	1.38
1	B	42	MET	CA-CB	5.36	1.63	1.53
1	B	39	PRO	C-N	-5.36	1.25	1.33
1	A	91	ILE	N-CA	-5.34	1.39	1.46
1	A	2	ILE	C-N	5.33	1.41	1.33
1	B	47	TRP	NE1-CE2	5.33	1.43	1.37
1	A	128	TYR	CA-C	5.31	1.58	1.52
1	A	110	LEU	N-CA	5.30	1.52	1.46
1	A	134	GLU	CA-C	5.30	1.59	1.52
1	A	24	LEU	CB-CG	5.29	1.64	1.53
1	B	129	GLU	C-O	-5.29	1.17	1.24
1	A	78	VAL	CB-CG2	5.29	1.70	1.52
1	A	93	VAL	CA-C	5.29	1.59	1.52
1	A	23	ASN	CA-C	5.28	1.59	1.53
1	B	142	ASP	CA-C	5.28	1.60	1.53
1	B	79	ASP	CG-OD1	5.28	1.35	1.25
1	A	55	PRO	CA-C	-5.27	1.45	1.52
1	A	98	ARG	CZ-NH2	5.27	1.40	1.33
1	B	98	ARG	CD-NE	-5.26	1.38	1.46
1	A	136	VAL	N-CA	5.25	1.52	1.46
1	B	149	HIS	CA-CB	-5.25	1.44	1.54
1	B	35	THR	CA-C	5.22	1.59	1.52
1	B	52	ARG	C-O	5.21	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	THR	N-CA	-5.20	1.39	1.46
1	A	114	HIS	CD2-NE2	5.20	1.43	1.37
1	A	30	TRP	CZ2-CH2	-5.19	1.27	1.37
1	A	90	GLU	N-CA	-5.18	1.40	1.46
1	B	124	HIS	CE1-NE2	5.17	1.37	1.32
1	B	28	LEU	CA-CB	5.16	1.61	1.53
1	B	84	ALA	C-N	-5.16	1.26	1.33
1	B	139	GLU	CA-C	5.15	1.58	1.52
1	A	78	VAL	C-N	5.13	1.40	1.33
1	B	49	SER	C-N	-5.13	1.27	1.33
1	B	36	LEU	CA-C	-5.12	1.46	1.52
1	A	86	GLY	N-CA	5.10	1.53	1.45
1	A	79	ASP	C-N	-5.09	1.26	1.33
1	B	7	ALA	CA-CB	5.09	1.60	1.53
1	B	156	LEU	C-O	-5.08	1.17	1.23
1	A	132	ASP	CA-CB	5.07	1.60	1.53
1	B	9	ALA	C-N	5.07	1.40	1.33
1	B	101	GLU	N-CA	5.06	1.52	1.46
1	B	49	SER	CB-OG	5.06	1.52	1.42
1	A	49	SER	C-O	5.05	1.30	1.24
1	A	92	MET	CA-CB	5.04	1.60	1.53
1	A	3	SER	CB-OG	5.03	1.52	1.42
1	A	67	GLY	C-O	5.03	1.30	1.23
1	B	11	ASP	CA-CB	5.03	1.61	1.53
1	B	139	GLU	C-N	5.02	1.40	1.33
1	A	61	ILE	C-N	-5.01	1.25	1.33
1	A	76	LYS	C-O	5.01	1.30	1.23
1	B	85	CYS	N-CA	5.01	1.52	1.46
1	A	1	MET	C-O	-5.00	1.13	1.23

All (885) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ASN	OD1-CG-ND2	-26.21	96.39	122.60
1	B	18	ASN	OD1-CG-ND2	25.60	148.20	122.60
1	B	158	ARG	CD-NE-CZ	23.88	157.83	124.40
1	B	120	GLU	CB-CG-CD	21.41	149.00	112.60
1	B	52	ARG	CD-NE-CZ	21.37	154.32	124.40
1	A	108	GLN	CA-CB-CG	19.73	153.56	114.10
1	B	38	LYS	O-C-N	19.59	138.65	121.80
1	B	81	ALA	CA-C-O	-19.57	100.54	120.70
1	A	52	ARG	CB-CG-CD	18.70	154.31	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	PRO	O-C-N	-18.26	102.01	123.01
1	B	111	TYR	CA-C-O	18.03	139.33	120.40
1	B	72	VAL	CA-C-O	-17.91	103.40	121.67
1	A	79	ASP	CA-C-O	-17.52	101.98	120.55
1	A	30	TRP	CA-C-O	-17.12	103.07	120.70
1	B	50	ILE	CA-C-O	-16.68	102.86	120.71
1	B	52	ARG	CB-CG-CD	16.66	149.61	111.30
1	B	12	ARG	CD-NE-CZ	16.52	147.53	124.40
1	B	59	ASN	OD1-CG-ND2	-16.44	106.16	122.60
1	B	38	LYS	CA-C-N	-16.31	102.38	119.99
1	B	38	LYS	C-N-CA	-16.31	102.38	119.99
1	B	101	GLU	O-C-N	-15.98	105.18	122.12
1	A	57	ARG	NE-CZ-NH1	15.67	137.17	121.50
1	B	71	ARG	NE-CZ-NH2	-15.66	105.11	119.20
1	B	87	ASP	CB-CG-OD2	-15.44	82.89	118.40
1	A	79	ASP	O-C-N	15.42	138.47	122.12
1	B	44	ARG	N-CA-C	15.41	127.66	111.17
1	B	111	TYR	O-C-N	-15.20	103.05	123.12
1	A	18	ASN	OD1-CG-ND2	15.10	137.70	122.60
1	B	33	ARG	CA-C-O	15.07	137.02	120.90
1	B	1	MET	O-C-N	14.85	146.75	123.00
1	B	135	SER	O-C-N	-14.82	104.29	122.96
1	A	98	ARG	NE-CZ-NH1	14.79	136.29	121.50
1	A	98	ARG	NE-CZ-NH2	-14.77	105.91	119.20
1	B	55	PRO	CA-C-O	-14.73	105.47	121.23
1	B	93	VAL	O-C-N	-14.65	106.25	122.95
1	B	52	ARG	CG-CD-NE	14.64	144.22	112.00
1	A	125	PHE	CA-C-O	-14.48	107.55	119.71
1	B	50	ILE	O-C-N	14.45	140.92	121.84
1	A	6	ALA	O-C-N	-14.20	107.58	123.48
1	B	6	ALA	O-C-N	-14.15	107.34	123.33
1	B	44	ARG	CA-C-O	14.15	135.54	120.69
1	B	88	VAL	CA-C-N	-14.11	104.23	119.19
1	B	88	VAL	C-N-CA	-14.11	104.23	119.19
1	A	143	ALA	CA-C-N	14.03	146.34	122.20
1	A	143	ALA	C-N-CA	14.03	146.34	122.20
1	B	9	ALA	CA-C-O	13.95	137.64	121.88
1	B	65	GLN	OE1-CD-NE2	-13.93	108.67	122.60
1	A	109	LYS	CA-CB-CG	13.86	141.83	114.10
1	B	73	THR	CA-CB-CG2	13.87	134.07	110.50
1	A	69	ASP	CA-C-O	13.86	136.19	120.80
1	B	37	ASP	CB-CG-OD2	-13.83	86.59	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	LYS	CG-CD-CE	-13.74	79.69	111.30
1	A	43	GLY	O-C-N	-13.74	109.83	122.88
1	B	1	MET	CA-C-N	-13.73	105.39	123.10
1	B	1	MET	C-N-CA	-13.73	105.39	123.10
1	B	55	PRO	N-CA-C	13.72	132.16	111.03
1	B	158	ARG	O-C-N	13.71	139.95	122.95
1	B	18	ASN	CB-CG-ND2	-13.63	95.96	116.40
1	A	87	ASP	CA-CB-CG	-13.62	98.98	112.60
1	B	67	GLY	N-CA-C	13.59	130.02	111.54
1	A	47	TRP	CA-C-O	13.57	135.99	121.07
1	A	16	MET	CG-SD-CE	13.54	130.68	100.90
1	B	118	GLU	CB-CG-CD	13.52	135.58	112.60
1	A	71	ARG	NE-CZ-NH2	13.51	131.35	119.20
1	A	135	SER	N-CA-CB	13.45	130.43	109.71
1	A	95	GLY	CA-C-N	13.41	145.85	121.70
1	A	95	GLY	C-N-CA	13.41	145.85	121.70
1	B	159	ARG	NE-CZ-NH2	-13.33	107.20	119.20
1	A	125	PHE	O-C-N	13.16	132.17	121.38
1	A	109	LYS	CB-CG-CD	12.98	141.16	111.30
1	B	104	LEU	CA-C-N	-12.93	107.15	119.82
1	B	104	LEU	C-N-CA	-12.93	107.15	119.82
1	A	22	TRP	CH2-CZ2-CE2	-12.80	100.86	117.50
1	A	145	ALA	O-C-N	12.74	137.13	122.22
1	B	118	GLU	CA-C-O	12.68	134.03	120.46
1	A	141	HIS	CE1-NE2-CD2	12.47	121.47	109.00
1	B	93	VAL	CA-C-N	12.39	141.15	122.69
1	B	93	VAL	C-N-CA	12.39	141.15	122.69
1	B	101	GLU	CA-CB-CG	12.38	138.85	114.10
1	A	57	ARG	NE-CZ-NH2	-12.36	108.08	119.20
1	B	6	ALA	CA-C-N	12.34	139.75	122.72
1	B	6	ALA	C-N-CA	12.34	139.75	122.72
1	B	59	ASN	CA-C-O	-12.34	106.66	120.60
1	A	44	ARG	CB-CG-CD	12.28	139.54	111.30
1	B	59	ASN	CA-C-N	12.24	138.37	123.19
1	B	59	ASN	C-N-CA	12.24	138.37	123.19
1	B	74	TRP	CE3-CZ3-CH2	-12.24	105.19	121.10
1	B	81	ALA	N-CA-C	-12.18	97.98	111.14
1	B	108	GLN	OE1-CD-NE2	-12.18	110.42	122.60
1	A	22	TRP	CD2-CE2-CZ2	12.16	134.56	122.40
1	B	54	LEU	O-C-N	12.15	133.43	121.28
1	A	81	ALA	CA-C-O	-12.09	108.25	120.70
1	B	31	PHE	CA-C-O	-12.07	107.80	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	VAL	CA-CB-CG1	12.06	130.90	110.40
1	B	42	MET	O-C-N	12.05	136.98	123.25
1	B	146	GLN	CG-CD-NE2	12.00	134.40	116.40
1	B	121	GLY	O-C-N	11.94	133.98	123.59
1	A	143	ALA	O-C-N	-11.93	108.80	122.75
1	B	101	GLU	CA-C-O	11.83	133.09	120.55
1	B	54	LEU	CA-C-N	-11.82	107.07	119.83
1	B	54	LEU	C-N-CA	-11.82	107.07	119.83
1	A	105	PRO	CA-C-O	11.65	135.84	119.18
1	A	141	HIS	CG-CD2-NE2	-11.65	95.55	107.20
1	A	150	SER	O-C-N	-11.61	108.53	122.81
1	A	82	ILE	N-CA-CB	11.60	123.39	110.51
1	A	120	GLU	CB-CG-CD	11.58	132.28	112.60
1	A	158	ARG	O-C-N	11.57	138.39	122.77
1	B	100	TYR	CB-CG-CD2	-11.56	103.46	120.80
1	B	52	ARG	NE-CZ-NH1	11.56	133.06	121.50
1	A	112	LEU	CA-C-O	11.44	133.06	120.70
1	B	151	TYR	CA-C-O	-11.42	108.20	120.99
1	B	141	HIS	ND1-CG-CD2	11.25	117.35	106.10
1	A	65	GLN	CB-CA-C	11.23	132.30	110.17
1	B	26	ALA	CA-C-O	11.23	132.45	120.55
1	B	31	PHE	O-C-N	11.21	134.07	122.08
1	B	61	ILE	N-CA-CB	11.16	126.14	111.64
1	B	69	ASP	CA-CB-CG	11.12	123.72	112.60
1	A	141	HIS	ND1-CG-CD2	11.11	117.21	106.10
1	B	120	GLU	CA-C-N	-11.00	110.47	122.57
1	B	120	GLU	C-N-CA	-11.00	110.47	122.57
1	A	45	HIS	CE1-NE2-CD2	10.97	119.97	109.00
1	A	107	ALA	CA-C-O	10.96	133.55	121.05
1	A	155	ILE	N-CA-CB	10.93	125.85	111.64
1	B	44	ARG	O-C-N	-10.85	110.62	122.12
1	A	71	ARG	CG-CD-NE	10.82	135.81	112.00
1	A	120	GLU	CA-CB-CG	10.82	135.74	114.10
1	B	141	HIS	CG-CD2-NE2	-10.81	96.39	107.20
1	A	22	TRP	NE1-CE2-CZ2	-10.79	113.92	130.10
1	B	53	PRO	CA-C-O	10.76	134.22	121.31
1	A	65	GLN	O-C-N	-10.76	108.95	121.32
1	A	100	TYR	O-C-N	10.73	133.50	122.12
1	A	73	THR	CA-CB-CG2	10.69	128.68	110.50
1	B	28	LEU	CA-C-O	-10.67	109.24	120.55
1	A	151	TYR	CA-C-N	10.65	138.62	123.07
1	A	151	TYR	C-N-CA	10.65	138.62	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	GLU	O-C-N	-10.65	109.71	123.13
1	A	78	VAL	CA-CB-CG1	10.61	128.44	110.40
1	B	60	ILE	CB-CA-C	10.59	126.61	110.83
1	A	69	ASP	N-CA-C	10.56	127.07	109.76
1	A	12	ARG	NE-CZ-NH2	10.56	128.70	119.20
1	B	9	ALA	O-C-N	-10.53	108.22	122.23
1	B	149	HIS	CA-CB-CG	10.53	124.33	113.80
1	B	17	GLU	OE1-CD-OE2	10.51	148.12	122.90
1	A	152	CYS	CA-C-N	10.49	136.50	121.50
1	A	152	CYS	C-N-CA	10.49	136.50	121.50
1	A	78	VAL	CA-C-O	10.40	133.79	120.78
1	A	157	GLU	CB-CG-CD	10.39	130.26	112.60
1	A	142	ASP	O-C-N	10.39	134.70	122.96
1	B	23	ASN	CA-CB-CG	-10.37	102.23	112.60
1	A	44	ARG	NE-CZ-NH1	10.35	131.85	121.50
1	A	87	ASP	CA-C-O	10.34	133.60	120.57
1	A	55	PRO	O-C-N	-10.31	110.14	123.13
1	A	82	ILE	CA-CB-CG2	10.30	128.00	110.50
1	A	72	VAL	CA-C-O	-10.27	111.46	121.63
1	A	95	GLY	N-CA-C	10.25	124.95	111.52
1	B	23	ASN	O-C-N	10.25	138.56	122.99
1	B	5	ILE	CB-CA-C	10.16	125.67	110.63
1	B	74	TRP	CZ3-CH2-CZ2	10.15	134.70	121.50
1	A	111	TYR	O-C-N	-10.14	110.39	122.87
1	A	153	PHE	CA-C-O	-10.14	109.13	120.69
1	A	85	CYS	CA-C-N	-10.11	104.01	121.39
1	A	85	CYS	C-N-CA	-10.11	104.01	121.39
1	B	153	PHE	CA-C-O	-10.09	109.14	120.54
1	B	7	ALA	CA-C-O	-10.08	109.44	120.43
1	A	109	LYS	CA-C-N	10.07	137.20	123.00
1	A	109	LYS	C-N-CA	10.07	137.20	123.00
1	A	21	PRO	N-CA-CB	10.05	109.49	102.35
1	A	45	HIS	ND1-CE1-NE2	-10.03	98.37	108.40
1	A	158	ARG	NE-CZ-NH1	10.02	131.52	121.50
1	B	23	ASN	CB-CG-OD1	10.02	140.84	120.80
1	B	108	GLN	CA-C-O	9.99	130.12	119.14
1	B	37	ASP	CB-CG-OD1	9.98	141.36	118.40
1	B	53	PRO	O-C-N	-9.97	111.13	123.10
1	B	60	ILE	CA-C-O	-9.97	109.91	120.48
1	A	113	THR	CA-C-O	-9.97	109.80	120.46
1	B	118	GLU	CG-CD-OE2	9.95	141.28	118.40
1	B	61	ILE	CA-CB-CG1	9.92	127.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TYR	CA-C-N	9.87	137.74	122.94
1	A	111	TYR	C-N-CA	9.87	137.74	122.94
1	B	141	HIS	CA-C-O	9.87	132.44	120.60
1	B	17	GLU	CB-CG-CD	9.84	129.32	112.60
1	A	116	ASP	CB-CG-OD1	9.84	141.02	118.40
1	A	144	ASP	N-CA-C	9.75	120.73	108.45
1	A	6	ALA	CA-C-O	9.70	131.56	120.89
1	A	71	ARG	CD-NE-CZ	9.68	137.96	124.40
1	A	58	LYS	CA-C-O	-9.68	109.66	120.60
1	A	111	TYR	CA-C-O	-9.68	110.39	120.84
1	A	44	ARG	CD-NE-CZ	-9.67	110.86	124.40
1	A	144	ASP	CA-C-N	9.67	134.20	120.28
1	A	144	ASP	C-N-CA	9.67	134.20	120.28
1	A	76	LYS	CA-C-O	-9.65	108.65	118.97
1	A	14	ILE	CA-C-O	-9.64	111.45	121.67
1	B	16	MET	CA-C-O	9.62	133.03	121.68
1	B	9	ALA	N-CA-C	-9.60	97.10	110.35
1	B	55	PRO	CA-C-N	9.59	138.24	121.07
1	B	55	PRO	C-N-CA	9.59	138.24	121.07
1	B	89	PRO	N-CA-C	9.58	126.12	113.57
1	B	159	ARG	CD-NE-CZ	-9.56	111.01	124.40
1	A	124	HIS	CA-C-N	9.51	134.43	120.83
1	A	124	HIS	C-N-CA	9.51	134.43	120.83
1	A	144	ASP	O-C-N	-9.50	110.48	122.73
1	B	48	GLU	CB-CG-CD	9.49	128.73	112.60
1	A	29	ALA	O-C-N	-9.45	112.11	122.12
1	B	126	PRO	CA-C-O	9.43	133.18	121.67
1	B	30	TRP	O-C-N	-9.41	111.92	122.09
1	B	140	PHE	CA-C-O	9.40	131.78	121.16
1	A	83	ALA	CA-C-O	-9.38	110.47	120.42
1	B	65	GLN	CB-CA-C	9.35	126.36	109.45
1	B	1	MET	CA-C-O	-9.34	104.93	120.80
1	A	110	LEU	CA-C-O	9.33	130.29	120.30
1	B	151	TYR	N-CA-C	9.33	123.64	108.99
1	B	46	THR	CA-C-O	-9.32	110.97	120.76
1	A	146	GLN	N-CA-CB	-9.29	96.88	110.53
1	A	121	GLY	CA-C-N	-9.28	104.45	121.52
1	A	121	GLY	C-N-CA	-9.28	104.45	121.52
1	A	82	ILE	CA-C-O	9.25	130.89	121.27
1	A	88	VAL	O-C-N	9.24	129.79	121.57
1	A	150	SER	CA-C-O	9.22	131.33	121.55
1	B	30	TRP	CA-C-N	9.20	133.58	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	TRP	C-N-CA	9.20	133.58	120.79
1	B	146	GLN	OE1-CD-NE2	-9.18	113.42	122.60
1	A	127	ASP	CB-CG-OD1	9.17	139.49	118.40
1	B	69	ASP	CB-CG-OD1	9.16	139.47	118.40
1	A	105	PRO	CA-CB-CG	9.12	121.83	104.50
1	B	119	VAL	CA-CB-CG1	-9.11	94.91	110.40
1	A	146	GLN	OE1-CD-NE2	9.09	131.69	122.60
1	B	68	THR	O-C-N	-9.08	111.49	122.48
1	A	48	GLU	CG-CD-OE2	-9.07	97.53	118.40
1	A	32	LYS	O-C-N	9.07	132.49	122.15
1	B	156	LEU	CB-CG-CD2	9.06	137.89	110.70
1	B	90	GLU	CA-C-O	9.06	132.44	120.21
1	B	50	ILE	CA-C-N	-9.04	103.70	121.41
1	B	50	ILE	C-N-CA	-9.04	103.70	121.41
1	B	23	ASN	CA-C-N	-9.03	112.22	123.15
1	B	23	ASN	C-N-CA	-9.03	112.22	123.15
1	A	74	TRP	O-C-N	-9.03	112.10	122.93
1	B	74	TRP	CD2-CE3-CZ3	9.02	130.33	118.60
1	B	20	MET	CA-C-O	9.01	129.54	120.17
1	B	29	ALA	CA-C-O	-8.98	109.64	119.97
1	B	154	LYS	CA-C-O	-8.97	110.34	120.66
1	A	23	ASN	CB-CG-OD1	8.96	138.72	120.80
1	A	147	ASN	OD1-CG-ND2	-8.94	113.66	122.60
1	A	65	GLN	CA-C-N	8.91	130.98	119.84
1	A	65	GLN	C-N-CA	8.91	130.98	119.84
1	A	159	ARG	CA-CB-CG	8.91	131.91	114.10
1	A	79	ASP	CA-CB-CG	-8.90	103.70	112.60
1	A	30	TRP	N-CA-C	-8.90	101.53	111.14
1	A	142	ASP	CA-C-O	-8.89	111.25	121.47
1	B	65	GLN	CA-C-O	8.88	130.87	120.92
1	A	133	TRP	CA-C-N	8.87	134.28	122.30
1	A	133	TRP	C-N-CA	8.87	134.28	122.30
1	B	87	ASP	OD1-CG-OD2	8.85	144.14	122.90
1	A	136	VAL	CA-CB-CG1	8.83	125.41	110.40
1	A	10	VAL	O-C-N	-8.81	111.56	122.57
1	A	54	LEU	O-C-N	8.80	130.75	121.42
1	B	20	MET	O-C-N	-8.79	112.24	121.30
1	B	29	ALA	CA-C-N	8.79	132.40	120.44
1	B	29	ALA	C-N-CA	8.79	132.40	120.44
1	A	44	ARG	CA-C-O	-8.78	109.43	119.79
1	B	44	ARG	NE-CZ-NH2	-8.78	111.30	119.20
1	B	17	GLU	CA-CB-CG	8.76	131.62	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	GLU	CA-C-O	8.76	130.04	119.97
1	A	14	ILE	O-C-N	8.76	132.16	122.97
1	A	18	ASN	CB-CG-ND2	-8.74	103.28	116.40
1	B	98	ARG	NE-CZ-NH2	8.73	127.05	119.20
1	B	94	ILE	N-CA-C	8.70	121.25	112.90
1	B	158	ARG	NE-CZ-NH2	8.66	127.00	119.20
1	A	22	TRP	CG-CD2-CE3	-8.62	125.28	133.90
1	B	51	GLY	O-C-N	-8.60	111.52	122.70
1	A	71	ARG	NH1-CZ-NH2	-8.58	108.15	119.30
1	A	69	ASP	N-CA-CB	-8.57	96.38	110.52
1	A	48	GLU	O-C-N	-8.57	111.73	122.27
1	A	55	PRO	CA-C-N	8.54	137.72	120.80
1	A	55	PRO	C-N-CA	8.54	137.72	120.80
1	B	114	HIS	CA-C-O	-8.53	110.88	120.43
1	B	115	ILE	O-C-N	8.53	131.84	123.14
1	B	17	GLU	CA-C-O	8.51	129.76	119.97
1	B	92	MET	CA-C-O	-8.50	111.26	120.36
1	B	53	PRO	N-CA-CB	8.50	111.24	103.34
1	B	137	PHE	O-C-N	8.48	132.85	123.52
1	A	21	PRO	N-CD-CG	8.48	115.92	103.20
1	A	23	ASN	CB-CG-ND2	-8.47	103.70	116.40
1	B	22	TRP	CZ3-CH2-CZ2	8.45	132.49	121.50
1	B	98	ARG	CG-CD-NE	8.44	130.58	112.00
1	B	5	ILE	CA-CB-CG1	-8.44	96.05	110.40
1	B	79	ASP	CA-C-O	-8.40	110.61	120.10
1	A	61	ILE	CA-CB-CG1	8.40	124.68	110.40
1	A	139	GLU	CG-CD-OE1	8.40	137.72	118.40
1	A	141	HIS	O-C-N	-8.37	113.20	123.33
1	A	22	TRP	CD2-CE3-CZ3	-8.33	107.78	118.60
1	B	118	GLU	OE1-CD-OE2	-8.32	102.93	122.90
1	B	133	TRP	CD2-CE2-CZ2	-8.31	114.09	122.40
1	A	14	ILE	CA-C-N	-8.26	111.19	120.53
1	A	14	ILE	C-N-CA	-8.26	111.19	120.53
1	B	29	ALA	N-CA-C	-8.26	102.23	111.82
1	A	147	ASN	CA-C-N	8.24	132.15	120.28
1	A	147	ASN	C-N-CA	8.24	132.15	120.28
1	B	10	VAL	CG1-CB-CG2	-8.21	92.74	110.80
1	A	23	ASN	CA-CB-CG	-8.20	104.40	112.60
1	A	55	PRO	CA-C-O	-8.18	111.88	121.86
1	B	48	GLU	CA-CB-CG	8.17	130.44	114.10
1	A	98	ARG	CA-C-O	8.15	129.19	120.55
1	A	156	LEU	O-C-N	-8.13	113.62	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	SER	CA-C-N	8.13	134.80	122.69
1	B	135	SER	C-N-CA	8.13	134.80	122.69
1	A	40	VAL	O-C-N	8.10	132.01	123.26
1	B	62	LEU	CA-C-O	8.10	128.96	120.54
1	A	149	HIS	CB-CG-CD2	-8.10	120.68	131.20
1	B	52	ARG	CA-CB-CG	8.08	130.27	114.10
1	A	155	ILE	CA-C-O	-8.06	112.00	120.39
1	A	46	THR	N-CA-CB	8.05	121.69	110.01
1	A	105	PRO	O-C-N	-8.05	111.45	122.24
1	A	150	SER	CA-C-N	8.05	137.08	121.63
1	A	150	SER	C-N-CA	8.05	137.08	121.63
1	B	158	ARG	NH1-CZ-NH2	-8.04	108.85	119.30
1	B	16	MET	CA-CB-CG	-8.03	98.03	114.10
1	A	21	PRO	CA-N-CD	-8.01	100.78	112.00
1	B	40	VAL	CA-C-O	-7.99	112.02	120.57
1	A	74	TRP	CA-C-N	7.99	136.08	122.67
1	A	74	TRP	C-N-CA	7.99	136.08	122.67
1	B	59	ASN	CA-CB-CG	7.97	120.57	112.60
1	B	98	ARG	NH1-CZ-NH2	-7.97	108.93	119.30
1	B	52	ARG	NH1-CZ-NH2	-7.97	108.94	119.30
1	B	53	PRO	CB-CA-C	-7.95	100.63	111.21
1	B	79	ASP	O-C-N	-7.95	112.91	122.22
1	B	127	ASP	CA-C-O	-7.95	111.67	120.81
1	A	126	PRO	CA-C-N	7.94	132.86	121.50
1	A	126	PRO	C-N-CA	7.94	132.86	121.50
1	B	124	HIS	CB-CG-CD2	-7.93	120.89	131.20
1	A	29	ALA	CA-C-N	7.92	131.21	120.44
1	A	29	ALA	C-N-CA	7.92	131.21	120.44
1	A	114	HIS	N-CA-CB	7.91	123.42	110.37
1	B	58	LYS	CA-C-O	7.89	128.81	120.36
1	A	40	VAL	CA-C-O	-7.87	112.12	120.39
1	B	1	MET	CA-CB-CG	7.86	129.83	114.10
1	A	89	PRO	CB-CA-C	-7.86	98.66	111.31
1	B	65	GLN	CG-CD-OE1	7.85	136.50	120.80
1	A	38	LYS	CA-CB-CG	7.84	129.78	114.10
1	B	8	LEU	O-C-N	-7.81	114.17	123.31
1	A	127	ASP	CB-CA-C	-7.81	97.11	109.84
1	B	105	PRO	CA-N-CD	-7.80	101.07	112.00
1	A	122	ASP	CA-CB-CG	-7.80	104.80	112.60
1	A	47	TRP	CA-C-N	-7.78	108.48	120.31
1	A	47	TRP	C-N-CA	-7.78	108.48	120.31
1	A	54	LEU	CA-C-N	-7.78	111.89	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	C-N-CA	-7.78	111.89	120.14
1	B	149	HIS	CA-C-O	-7.76	112.64	121.40
1	A	100	TYR	CG-CD1-CE1	-7.73	109.61	121.20
1	B	57	ARG	CA-CB-CG	-7.73	98.65	114.10
1	A	135	SER	CB-CA-C	-7.71	98.69	110.26
1	B	89	PRO	N-CA-CB	-7.70	95.36	103.52
1	A	88	VAL	CA-C-N	-7.69	111.88	119.64
1	A	88	VAL	C-N-CA	-7.69	111.88	119.64
1	B	14	ILE	N-CA-CB	7.68	122.49	112.12
1	B	110	LEU	CA-C-O	-7.67	111.80	120.32
1	A	30	TRP	CA-C-N	7.67	130.41	120.44
1	A	30	TRP	C-N-CA	7.67	130.41	120.44
1	A	152	CYS	O-C-N	-7.66	113.02	123.12
1	A	11	ASP	CA-C-O	7.65	128.92	120.12
1	A	27	ASP	CA-C-O	-7.64	111.75	120.24
1	A	69	ASP	CB-CG-OD2	-7.64	100.82	118.40
1	B	1	MET	CB-CG-SD	7.63	135.58	112.70
1	B	131	ASP	N-CA-C	-7.62	103.96	113.18
1	B	145	ALA	CA-C-O	-7.62	110.27	119.49
1	A	10	VAL	CA-CB-CG1	7.61	123.33	110.40
1	A	158	ARG	CB-CA-C	-7.61	99.11	110.67
1	A	35	THR	CA-C-O	-7.59	110.85	118.97
1	B	25	PRO	CA-C-O	7.58	131.08	119.55
1	A	48	GLU	CB-CA-C	-7.58	96.12	110.67
1	B	57	ARG	N-CA-CB	-7.58	98.50	111.69
1	A	131	ASP	CB-CA-C	-7.58	94.87	109.95
1	A	134	GLU	O-C-N	-7.57	114.43	123.13
1	B	157	GLU	CG-CD-OE2	-7.57	100.99	118.40
1	B	101	GLU	CG-CD-OE2	-7.57	101.00	118.40
1	A	130	PRO	N-CA-CB	7.56	111.19	103.25
1	A	140	PHE	O-C-N	7.55	131.78	123.10
1	B	62	LEU	CD1-CG-CD2	-7.54	94.21	110.80
1	A	132	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	147	ASN	CB-CG-OD1	7.53	135.86	120.80
1	A	111	TYR	CG-CD1-CE1	-7.52	109.92	121.20
1	B	33	ARG	NE-CZ-NH1	7.52	129.02	121.50
1	A	31	PHE	CA-C-N	-7.52	109.62	120.29
1	A	31	PHE	C-N-CA	-7.52	109.62	120.29
1	B	27	ASP	CA-C-O	-7.50	112.94	120.82
1	B	146	GLN	CB-CG-CD	-7.50	99.85	112.60
1	A	10	VAL	CG1-CB-CG2	-7.50	94.31	110.80
1	B	4	LEU	CA-C-O	-7.48	112.28	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45[A]	HIS	O-C-N	-7.47	113.64	122.15
1	B	45[B]	HIS	O-C-N	-7.47	113.64	122.15
1	A	46	THR	CA-CB-OG1	-7.46	98.41	109.60
1	A	62	LEU	O-C-N	-7.44	114.20	123.05
1	B	80	GLU	N-CA-CB	-7.44	98.75	110.28
1	A	14	ILE	N-CA-CB	7.43	122.19	112.60
1	B	158	ARG	CA-C-N	-7.43	108.33	121.70
1	B	158	ARG	C-N-CA	-7.43	108.33	121.70
1	A	12	ARG	CD-NE-CZ	7.42	134.79	124.40
1	B	141	HIS	O-C-N	-7.41	114.36	123.33
1	A	68	THR	O-C-N	-7.39	114.17	122.08
1	A	17	GLU	O-C-N	7.38	132.41	122.59
1	A	46	THR	CA-C-N	7.37	131.03	120.79
1	A	46	THR	C-N-CA	7.37	131.03	120.79
1	B	37	ASP	N-CA-C	7.37	121.67	112.24
1	A	31	PHE	O-C-N	7.37	129.66	122.07
1	B	106	LYS	CB-CG-CD	7.37	128.24	111.30
1	B	99	VAL	CA-C-O	7.36	128.60	120.95
1	A	25	PRO	O-C-N	-7.33	112.76	122.22
1	A	158	ARG	CG-CD-NE	-7.33	95.88	112.00
1	A	151	TYR	N-CA-C	7.32	120.33	108.76
1	B	18	ASN	CA-C-O	7.32	130.61	121.46
1	B	90	GLU	CB-CG-CD	7.32	125.04	112.60
1	B	100	TYR	CG-CD1-CE1	-7.30	110.25	121.20
1	A	12	ARG	CG-CD-NE	7.30	128.05	112.00
1	A	53	PRO	N-CA-CB	7.29	110.12	103.34
1	B	37	ASP	CA-CB-CG	-7.29	105.31	112.60
1	A	91	ILE	CA-C-O	-7.28	112.65	120.59
1	B	40	VAL	O-C-N	7.28	131.11	123.03
1	B	69	ASP	CB-CG-OD2	-7.28	101.66	118.40
1	A	60	ILE	CA-C-O	-7.28	112.82	120.39
1	A	118	GLU	CA-C-O	7.26	128.09	120.54
1	A	8	LEU	CB-CG-CD2	7.26	132.47	110.70
1	A	126	PRO	O-C-N	-7.26	112.84	122.64
1	A	22	TRP	CE3-CZ3-CH2	7.25	130.53	121.10
1	A	62	LEU	CA-C-O	7.25	128.07	120.54
1	B	16	MET	O-C-N	-7.24	112.59	122.94
1	B	22	TRP	CA-C-O	7.23	129.14	121.33
1	B	96	GLY	CA-C-O	7.23	135.98	120.80
1	B	111	TYR	CA-C-N	7.21	133.16	122.99
1	B	111	TYR	C-N-CA	7.21	133.16	122.99
1	A	81	ALA	CA-C-N	7.21	129.90	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ALA	C-N-CA	7.21	129.90	120.60
1	A	150	SER	CB-CA-C	7.21	122.52	109.62
1	B	47	TRP	N-CA-CB	-7.21	99.25	110.06
1	A	155	ILE	CA-CB-CG1	-7.18	98.19	110.40
1	B	39	PRO	CA-C-N	7.18	131.97	122.93
1	B	39	PRO	C-N-CA	7.18	131.97	122.93
1	B	42	MET	CA-C-N	-7.17	110.98	121.30
1	B	42	MET	C-N-CA	-7.17	110.98	121.30
1	A	81	ALA	N-CA-C	-7.17	103.40	111.14
1	B	30	TRP	CB-CG-CD1	7.16	137.63	126.90
1	B	112	LEU	O-C-N	7.15	131.81	123.30
1	B	25	PRO	O-C-N	-7.15	113.00	122.22
1	B	26	ALA	O-C-N	-7.15	114.55	122.12
1	B	42	MET	CA-C-O	-7.15	113.61	121.33
1	A	23	ASN	CA-C-O	-7.14	110.59	120.52
1	A	154	LYS	CG-CD-CE	7.13	127.70	111.30
1	A	143	ALA	CA-C-O	-7.12	114.03	121.87
1	B	7	ALA	CB-CA-C	7.12	121.49	109.75
1	A	132	ASP	N-CA-CB	-7.12	99.53	110.92
1	B	81	ALA	CA-C-N	7.11	129.52	120.56
1	B	81	ALA	C-N-CA	7.11	129.52	120.56
1	A	17	GLU	CA-C-O	-7.09	110.36	120.51
1	A	152	CYS	CA-C-O	-7.09	112.96	120.40
1	A	69	ASP	OD1-CG-OD2	7.09	139.91	122.90
1	A	22	TRP	CE2-CD2-CG	7.08	115.69	107.20
1	A	152	CYS	N-CA-C	7.08	120.40	108.02
1	A	119	VAL	CA-C-N	-7.07	112.22	122.19
1	A	119	VAL	C-N-CA	-7.07	112.22	122.19
1	A	103	PHE	O-C-N	-7.06	113.03	122.49
1	A	7	ALA	CA-C-O	7.06	127.81	120.40
1	B	72	VAL	N-CA-C	7.05	119.09	108.80
1	B	2	ILE	CA-CB-CG2	7.04	122.47	110.50
1	B	88	VAL	CA-CB-CG1	-7.03	98.44	110.40
1	B	138	SER	N-CA-CB	-7.03	98.40	111.13
1	B	62	LEU	N-CA-CB	7.03	121.97	110.37
1	B	68	THR	CA-CB-CG2	7.03	122.45	110.50
1	A	158	ARG	CB-CG-CD	-7.02	95.16	111.30
1	A	79	ASP	CB-CG-OD1	6.99	134.49	118.40
1	A	88	VAL	CA-CB-CG2	6.98	122.26	110.40
1	B	100	TYR	O-C-N	6.98	130.10	122.15
1	B	102	GLN	CA-C-O	6.97	127.81	120.42
1	A	95	GLY	CA-C-O	-6.96	115.25	122.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	MET	N-CA-CB	6.96	120.91	109.98
1	B	32	LYS	CA-C-N	6.95	129.93	120.54
1	B	32	LYS	C-N-CA	6.95	129.93	120.54
1	B	82	ILE	CB-CG1-CD1	6.95	128.39	113.80
1	B	58	LYS	CA-C-N	6.93	132.32	121.99
1	B	58	LYS	C-N-CA	6.93	132.32	121.99
1	B	17	GLU	CG-CD-OE2	-6.93	102.46	118.40
1	A	77	SER	CA-C-N	6.92	134.42	121.97
1	A	77	SER	C-N-CA	6.92	134.42	121.97
1	A	158	ARG	N-CA-CB	6.90	120.91	109.60
1	A	76	LYS	N-CA-C	-6.89	105.14	113.97
1	A	90	GLU	CG-CD-OE1	6.89	134.25	118.40
1	B	13	VAL	O-C-N	6.89	130.18	122.67
1	B	128	TYR	N-CA-C	-6.89	99.27	109.81
1	A	61	ILE	CB-CG1-CD1	6.88	128.25	113.80
1	B	41	ILE	O-C-N	-6.88	115.64	122.93
1	A	11	ASP	CB-CG-OD1	6.87	134.20	118.40
1	B	111	TYR	CB-CG-CD2	-6.85	110.52	120.80
1	A	109	LYS	CG-CD-CE	6.85	127.05	111.30
1	B	28	LEU	O-C-N	6.83	129.36	122.12
1	B	89	PRO	CA-N-CD	6.82	121.55	112.00
1	A	79	ASP	N-CA-CB	-6.81	100.11	110.12
1	B	39	PRO	N-CD-CG	6.80	113.40	103.20
1	B	52	ARG	N-CA-CB	-6.80	98.27	110.37
1	B	84	ALA	N-CA-CB	-6.79	98.50	110.39
1	A	154	LYS	CA-C-N	6.79	132.13	123.10
1	A	154	LYS	C-N-CA	6.79	132.13	123.10
1	A	30	TRP	CZ3-CH2-CZ2	6.77	130.30	121.50
1	B	84	ALA	CA-C-N	6.76	132.17	120.68
1	B	84	ALA	C-N-CA	6.76	132.17	120.68
1	B	3	SER	O-C-N	-6.75	115.03	123.27
1	B	71	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	B	7	ALA	CA-C-N	6.75	133.13	122.74
1	B	7	ALA	C-N-CA	6.75	133.13	122.74
1	A	48	GLU	N-CA-C	6.74	119.64	111.82
1	A	60	ILE	CA-C-N	6.74	132.28	123.11
1	A	60	ILE	C-N-CA	6.74	132.28	123.11
1	A	39	PRO	CB-CA-C	-6.74	100.99	110.63
1	B	154	LYS	CB-CG-CD	-6.73	95.83	111.30
1	A	120	GLU	O-C-N	-6.72	115.56	123.22
1	A	129	GLU	CB-CA-C	6.72	123.42	110.17
1	B	158	ARG	CA-C-O	-6.72	113.26	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ILE	N-CA-CB	6.70	119.05	111.21
1	B	114	HIS	O-C-N	-6.69	115.43	123.13
1	B	114	HIS	CA-C-N	6.69	131.73	123.10
1	B	114	HIS	C-N-CA	6.69	131.73	123.10
1	B	123	THR	CA-CB-CG2	6.68	121.86	110.50
1	B	40	VAL	CB-CA-C	6.68	119.93	110.84
1	B	7	ALA	O-C-N	-6.67	115.74	123.27
1	A	146	GLN	CG-CD-NE2	-6.66	106.41	116.40
1	B	86	GLY	O-C-N	6.65	131.35	122.70
1	A	145	ALA	CB-CA-C	6.63	122.90	110.63
1	B	115	ILE	CA-C-N	-6.63	112.22	122.16
1	B	115	ILE	C-N-CA	-6.63	112.22	122.16
1	A	1	MET	CG-SD-CE	6.61	115.45	100.90
1	A	48	GLU	CA-CB-CG	6.61	127.33	114.10
1	B	159	ARG	NH1-CZ-NH2	6.61	127.89	119.30
1	A	134	GLU	N-CA-C	6.60	119.45	108.96
1	B	100	TYR	CA-C-O	-6.59	113.43	120.42
1	A	44	ARG	NH1-CZ-NH2	-6.59	110.73	119.30
1	A	86	GLY	O-C-N	6.59	129.45	122.86
1	B	130	PRO	O-C-N	6.58	131.25	122.30
1	B	59	ASN	CB-CG-OD1	6.56	133.93	120.80
1	A	128	TYR	O-C-N	6.56	131.27	123.33
1	B	139	GLU	CG-CD-OE1	6.56	133.49	118.40
1	A	47	TRP	CG-CD2-CE3	6.55	140.45	133.90
1	A	80	GLU	N-CA-CB	-6.55	99.51	110.39
1	B	59	ASN	O-C-N	-6.55	114.30	122.82
1	B	27	ASP	CB-CG-OD1	6.55	133.46	118.40
1	A	78	VAL	CG1-CB-CG2	-6.53	96.43	110.80
1	B	132	ASP	O-C-N	6.53	130.81	122.39
1	A	111	TYR	CB-CG-CD2	-6.53	111.01	120.80
1	A	6	ALA	CA-C-N	6.52	132.59	123.07
1	A	6	ALA	C-N-CA	6.52	132.59	123.07
1	A	141	HIS	ND1-CE1-NE2	-6.51	101.89	108.40
1	A	118	GLU	O-C-N	-6.51	115.31	123.05
1	B	78	VAL	N-CA-CB	6.51	118.16	110.55
1	B	145	ALA	O-C-N	6.50	130.85	122.39
1	A	78	VAL	CA-C-N	-6.49	111.58	120.28
1	A	78	VAL	C-N-CA	-6.49	111.58	120.28
1	B	152	CYS	CA-C-O	-6.49	113.20	120.66
1	B	61	ILE	CA-CB-CG2	6.48	121.52	110.50
1	A	34	ASN	O-C-N	-6.48	113.43	122.37
1	B	61	ILE	CA-C-N	6.47	131.25	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ILE	C-N-CA	6.47	131.25	122.84
1	B	15	GLY	O-C-N	6.47	131.10	122.70
1	A	50	ILE	CA-C-O	6.46	128.22	121.05
1	B	88	VAL	CG1-CB-CG2	6.46	125.02	110.80
1	A	32	LYS	N-CA-CB	-6.45	100.61	110.16
1	B	65	GLN	N-CA-C	-6.45	100.72	110.40
1	A	30	TRP	CG-CD2-CE3	-6.45	127.45	133.90
1	B	147	ASN	O-C-N	-6.44	115.80	123.27
1	A	119	VAL	CA-C-O	-6.44	112.82	121.32
1	A	124	HIS	ND1-CE1-NE2	-6.43	101.97	108.40
1	A	104	LEU	CA-CB-CG	6.43	138.79	116.30
1	B	22	TRP	CH2-CZ2-CE2	-6.41	109.17	117.50
1	A	93	VAL	CA-C-O	-6.41	113.61	120.59
1	A	47	TRP	CD2-CE3-CZ3	6.39	126.91	118.60
1	A	72	VAL	CG1-CB-CG2	-6.39	96.74	110.80
1	B	105	PRO	CB-CG-CD	-6.39	85.66	106.10
1	B	130	PRO	N-CA-CB	6.39	109.64	103.51
1	B	40	VAL	CA-CB-CG1	6.38	121.25	110.40
1	B	46	THR	CA-CB-CG2	6.38	121.35	110.50
1	A	154	LYS	CB-CG-CD	6.38	125.97	111.30
1	A	57	ARG	CA-C-O	6.35	128.42	121.06
1	A	58	LYS	CA-CB-CG	-6.34	101.42	114.10
1	B	16	MET	N-CA-C	-6.34	100.11	109.81
1	B	32	LYS	O-C-N	-6.33	115.41	122.12
1	B	11	ASP	CA-C-N	-6.32	113.64	122.74
1	B	11	ASP	C-N-CA	-6.32	113.64	122.74
1	A	99	VAL	CB-CA-C	6.32	120.06	111.97
1	B	142	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	13	VAL	CA-C-O	-6.32	113.84	121.04
1	B	23	ASN	N-CA-CB	-6.31	100.58	110.87
1	B	87	ASP	CB-CG-OD1	6.30	132.89	118.40
1	B	76	LYS	N-CA-CB	-6.30	101.42	110.80
1	A	8	LEU	CA-C-O	6.29	127.24	120.38
1	A	66	PRO	CA-C-O	6.28	132.02	120.60
1	A	31	PHE	CG-CD2-CE2	-6.25	110.08	120.70
1	A	32	LYS	CA-C-N	-6.25	111.82	120.38
1	A	32	LYS	C-N-CA	-6.25	111.82	120.38
1	B	155	ILE	N-CA-C	-6.24	99.49	108.48
1	A	128	TYR	N-CA-C	-6.24	98.46	109.06
1	B	30	TRP	CB-CG-CD2	-6.24	118.07	126.80
1	A	4	LEU	N-CA-CB	6.23	120.73	110.69
1	A	7	ALA	O-C-N	-6.22	114.91	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	TRP	NE1-CE2-CZ2	6.22	139.43	130.10
1	B	80	GLU	OE1-CD-OE2	6.21	137.81	122.90
1	A	139	GLU	CG-CD-OE2	-6.21	104.11	118.40
1	A	74	TRP	CA-C-O	-6.20	113.94	120.58
1	B	142	ASP	OD1-CG-OD2	6.20	137.77	122.90
1	A	106	LYS	CA-C-O	6.19	126.52	119.27
1	B	61	ILE	N-CA-C	-6.19	98.71	107.75
1	B	61	ILE	CG1-CB-CG2	-6.18	92.15	110.70
1	B	84	ALA	N-CA-C	6.18	120.43	113.01
1	B	40	VAL	N-CA-C	6.18	117.19	108.36
1	A	5	ILE	O-C-N	6.18	129.71	123.10
1	B	11	ASP	CA-C-O	6.18	127.22	120.12
1	B	152	CYS	CA-C-N	6.16	130.88	122.19
1	B	152	CYS	C-N-CA	6.16	130.88	122.19
1	B	157	GLU	CA-CB-CG	6.16	126.41	114.10
1	B	36	LEU	O-C-N	-6.15	115.46	122.97
1	B	77	SER	O-C-N	6.14	130.60	123.17
1	B	121	GLY	CA-C-O	-6.14	114.83	121.82
1	B	34	ASN	CB-CG-OD1	6.14	133.07	120.80
1	B	53	PRO	CA-CB-CG	-6.12	92.87	104.50
1	A	145	ALA	CA-C-O	-6.12	113.19	120.10
1	A	52	ARG	CA-C-N	-6.11	113.65	119.76
1	A	52	ARG	C-N-CA	-6.11	113.65	119.76
1	A	90	GLU	CA-C-N	6.11	130.72	122.90
1	A	90	GLU	C-N-CA	6.11	130.72	122.90
1	B	44	ARG	CD-NE-CZ	-6.10	115.86	124.40
1	B	106	LYS	CA-C-O	6.10	126.41	119.27
1	A	69	ASP	O-C-N	-6.10	116.06	123.19
1	B	4	LEU	CB-CG-CD1	6.09	128.98	110.70
1	A	24	LEU	CA-C-O	6.09	127.98	121.28
1	B	38	LYS	N-CA-C	-6.09	99.65	109.58
1	B	103	PHE	O-C-N	6.09	130.86	122.46
1	B	68	THR	N-CA-C	-6.09	106.18	113.97
1	A	89	PRO	N-CA-C	6.08	122.63	114.18
1	A	147	ASN	CA-CB-CG	-6.08	106.53	112.60
1	A	19	ALA	CA-C-O	6.07	127.96	121.16
1	B	102	GLN	N-CA-CB	-6.06	101.19	110.16
1	B	140	PHE	CG-CD2-CE2	6.06	131.01	120.70
1	A	68	THR	CB-CA-C	6.06	120.55	110.92
1	A	92	MET	O-C-N	-6.06	116.31	123.22
1	A	33	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	98	ARG	CA-CB-CG	-6.05	102.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASP	CB-CG-OD2	-6.04	104.50	118.40
1	B	154	LYS	N-CA-C	6.04	119.33	109.24
1	A	36	LEU	CA-C-N	-6.03	114.09	124.82
1	A	36	LEU	C-N-CA	-6.03	114.09	124.82
1	A	37	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	25	PRO	CB-CA-C	-6.02	102.82	112.21
1	A	141	HIS	CA-C-N	6.01	131.37	121.39
1	A	141	HIS	C-N-CA	6.01	131.37	121.39
1	A	59	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	B	156	LEU	CA-C-O	6.00	127.56	120.66
1	B	100	TYR	CD1-CG-CD2	5.99	127.09	118.10
1	B	68	THR	CB-CA-C	5.99	119.13	109.07
1	A	48	GLU	OE1-CD-OE2	5.98	137.26	122.90
1	B	29	ALA	O-C-N	-5.98	114.92	122.27
1	B	94	ILE	CA-C-O	5.97	125.62	119.35
1	A	80	GLU	CB-CA-C	-5.97	97.83	110.31
1	A	114	HIS	CA-C-N	-5.97	115.39	123.10
1	A	114	HIS	C-N-CA	-5.97	115.39	123.10
1	A	45	HIS	CA-C-N	5.97	128.20	120.44
1	A	45	HIS	C-N-CA	5.97	128.20	120.44
1	A	73	THR	OG1-CB-CG2	5.96	121.23	109.30
1	B	146	GLN	CA-CB-CG	-5.96	102.17	114.10
1	B	116	ASP	N-CA-CB	-5.94	102.55	110.57
1	B	99	VAL	CA-C-N	-5.93	111.86	120.29
1	B	99	VAL	C-N-CA	-5.93	111.86	120.29
1	A	79	ASP	OD1-CG-OD2	-5.93	108.67	122.90
1	B	155	ILE	CA-C-O	5.92	127.60	120.67
1	B	127	ASP	O-C-N	5.92	130.21	122.93
1	B	147	ASN	CA-CB-CG	-5.92	106.68	112.60
1	B	49	SER	CA-CB-OG	-5.91	99.27	111.10
1	A	152	CYS	CB-CA-C	5.91	120.26	110.74
1	B	36	LEU	CB-CG-CD1	5.91	128.42	110.70
1	B	46	THR	N-CA-C	-5.90	104.79	111.10
1	B	30	TRP	NE1-CE2-CD2	-5.89	99.74	107.40
1	A	141	HIS	CB-CG-ND1	-5.88	113.87	122.70
1	B	18	ASN	N-CA-CB	-5.87	100.78	110.65
1	B	97	GLY	N-CA-C	5.87	127.09	113.18
1	B	33	ARG	O-C-N	-5.87	115.99	122.09
1	B	50	ILE	N-CA-C	-5.86	104.61	111.00
1	B	93	VAL	CA-C-O	-5.86	114.09	120.71
1	A	30	TRP	CE3-CZ3-CH2	-5.85	113.50	121.10
1	B	44	ARG	N-CA-CB	-5.84	101.59	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	MET	CG-SD-CE	5.84	113.74	100.90
1	A	140	PHE	CA-C-N	-5.83	112.34	122.37
1	A	140	PHE	C-N-CA	-5.83	112.34	122.37
1	B	88	VAL	CA-C-O	5.83	127.76	119.95
1	B	108	GLN	CG-CD-NE2	5.82	125.13	116.40
1	B	80	GLU	CA-C-O	5.82	126.66	119.97
1	A	109	LYS	O-C-N	5.81	130.01	123.27
1	B	105	PRO	N-CA-C	5.81	121.48	113.98
1	B	124	HIS	CB-CG-ND1	5.81	131.42	122.70
1	A	22	TRP	CD1-NE1-CE2	-5.79	98.48	108.90
1	A	88	VAL	N-CA-C	-5.79	101.50	108.45
1	A	71	ARG	N-CA-CB	-5.79	101.04	110.42
1	B	138	SER	O-C-N	-5.79	116.64	123.41
1	B	17	GLU	N-CA-CB	-5.79	101.31	110.28
1	B	79	ASP	OD1-CG-OD2	-5.79	109.01	122.90
1	A	111	TYR	CD1-CG-CD2	5.78	126.76	118.10
1	B	104	LEU	N-CA-CB	5.77	120.64	110.37
1	A	38	LYS	CB-CG-CD	5.76	124.55	111.30
1	B	100	TYR	CB-CG-CD1	5.76	129.44	120.80
1	B	113	THR	CA-CB-CG2	5.76	120.29	110.50
1	B	119	VAL	CG1-CB-CG2	5.75	123.45	110.80
1	A	61	ILE	O-C-N	5.74	130.40	122.88
1	B	104	LEU	C-N-CD	5.74	148.54	125.00
1	A	35	THR	CA-C-N	-5.74	112.72	120.87
1	A	35	THR	C-N-CA	-5.74	112.72	120.87
1	B	116	ASP	CB-CG-OD2	-5.74	105.20	118.40
1	B	30	TRP	NE1-CE2-CZ2	5.74	138.70	130.10
1	A	155	ILE	O-C-N	5.72	129.27	123.20
1	A	23	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	36	LEU	N-CA-CB	-5.72	101.56	109.97
1	A	51	GLY	N-CA-C	5.72	123.70	114.90
1	A	48	GLU	CB-CG-CD	5.71	122.31	112.60
1	B	13	VAL	CA-CB-CG2	-5.71	100.70	110.40
1	B	39	PRO	CB-CA-C	-5.70	102.81	110.85
1	B	22	TRP	O-C-N	-5.69	116.76	123.25
1	A	133	TRP	CD2-CE2-CZ2	5.68	128.08	122.40
1	B	133	TRP	CE3-CZ3-CH2	-5.67	113.72	121.10
1	A	2	ILE	CA-C-O	5.67	126.64	120.57
1	B	82	ILE	CA-C-N	-5.66	112.13	120.28
1	B	82	ILE	C-N-CA	-5.66	112.13	120.28
1	B	85	CYS	O-C-N	5.66	129.91	122.33
1	A	4	LEU	CB-CG-CD1	5.65	127.65	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	VAL	O-C-N	5.64	129.31	123.04
1	B	97	GLY	CA-C-O	5.64	130.39	120.57
1	A	103	PHE	CZ-CE2-CD2	-5.64	109.85	120.00
1	A	3	SER	O-C-N	5.63	130.51	123.19
1	A	103	PHE	CE1-CZ-CE2	5.63	130.13	120.00
1	A	49	SER	CA-C-O	-5.63	114.46	120.42
1	B	108	GLN	N-CA-CB	-5.62	102.26	110.53
1	A	88	VAL	CG1-CB-CG2	-5.62	98.45	110.80
1	A	109	LYS	CA-C-O	-5.62	114.55	121.06
1	A	68	THR	CA-C-N	5.61	131.00	122.65
1	A	68	THR	C-N-CA	5.61	131.00	122.65
1	B	34	ASN	CB-CG-ND2	-5.61	107.99	116.40
1	B	35	THR	N-CA-C	-5.61	107.08	114.31
1	A	69	ASP	CB-CA-C	5.60	118.88	109.48
1	B	12	ARG	CA-C-N	5.59	128.58	120.98
1	B	12	ARG	C-N-CA	5.59	128.58	120.98
1	B	82	ILE	CA-C-O	5.59	127.09	121.17
1	B	34	ASN	O-C-N	5.59	130.08	122.37
1	A	128	TYR	CA-C-O	5.58	127.30	120.60
1	A	22	TRP	CD1-CG-CD2	-5.58	97.38	106.30
1	B	59	ASN	N-CA-C	5.57	117.31	108.67
1	B	114	HIS	CB-CA-C	5.57	119.52	110.22
1	A	13	VAL	O-C-N	5.57	128.35	122.67
1	A	75	VAL	CA-C-O	5.56	128.66	121.32
1	B	2	ILE	CA-CB-CG1	-5.56	100.94	110.40
1	A	31	PHE	CB-CG-CD2	-5.56	111.25	120.70
1	A	49	SER	N-CA-C	-5.56	105.30	111.36
1	A	146	GLN	O-C-N	-5.56	115.04	122.49
1	B	27	ASP	CB-CG-OD2	-5.55	105.64	118.40
1	B	151	TYR	O-C-N	5.54	129.59	123.33
1	A	24	LEU	CA-C-N	-5.53	113.20	119.28
1	A	24	LEU	C-N-CA	-5.53	113.20	119.28
1	A	63	SER	O-C-N	5.53	129.33	123.42
1	B	85	CYS	N-CA-C	-5.52	105.28	112.23
1	A	151	TYR	O-C-N	-5.51	117.31	123.48
1	B	134	GLU	CG-CD-OE2	-5.51	105.73	118.40
1	B	46	THR	O-C-N	5.51	127.74	122.07
1	A	125	PHE	CA-C-N	-5.50	112.97	119.84
1	A	125	PHE	C-N-CA	-5.50	112.97	119.84
1	B	137	PHE	N-CA-C	-5.50	100.16	108.46
1	B	138	SER	CA-C-O	5.50	127.30	120.54
1	A	7	ALA	CA-C-N	5.49	130.58	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ALA	C-N-CA	5.49	130.58	123.00
1	A	70	ASP	O-C-N	5.49	130.04	122.46
1	B	72	VAL	CG1-CB-CG2	5.49	122.88	110.80
1	A	116	ASP	OD1-CG-OD2	-5.49	109.73	122.90
1	A	74	TRP	CD2-CE2-CZ2	5.49	127.89	122.40
1	B	26	ALA	N-CA-C	5.48	117.25	111.28
1	B	103	PHE	CZ-CE2-CD2	5.46	129.84	120.00
1	A	105	PRO	N-CA-CB	-5.46	98.02	103.48
1	B	38	LYS	C-N-CD	5.46	147.37	125.00
1	B	44	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	134	GLU	CA-C-N	5.44	129.07	121.24
1	A	134	GLU	C-N-CA	5.44	129.07	121.24
1	B	36	LEU	CA-C-N	5.44	130.28	122.40
1	B	36	LEU	C-N-CA	5.44	130.28	122.40
1	B	128	TYR	CA-C-N	5.44	131.22	121.76
1	B	128	TYR	C-N-CA	5.44	131.22	121.76
1	A	43	GLY	CA-C-O	-5.43	116.85	122.28
1	B	90	GLU	O-C-N	-5.43	116.76	123.44
1	A	17	GLU	CA-CB-CG	5.43	124.96	114.10
1	B	132	ASP	N-CA-CB	-5.42	102.61	110.47
1	A	31	PHE	CD1-CG-CD2	5.42	126.72	118.60
1	B	119	VAL	CA-CB-CG2	5.41	119.59	110.40
1	A	113	THR	CB-CA-C	5.40	119.59	110.79
1	A	159	ARG	CA-C-O	-5.39	104.82	121.00
1	A	128	TYR	CG-CD1-CE1	5.39	129.29	121.20
1	B	18	ASN	N-CA-C	-5.39	101.24	109.65
1	A	119	VAL	O-C-N	5.38	128.68	123.03
1	B	138	SER	CA-CB-OG	-5.38	100.33	111.10
1	B	14	ILE	CA-C-O	5.38	124.52	118.98
1	A	29	ALA	N-CA-CB	-5.37	102.22	110.12
1	A	46	THR	N-CA-C	-5.37	105.33	111.07
1	B	98	ARG	CB-CA-C	-5.36	99.44	110.38
1	B	71	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	B	128	TYR	CB-CG-CD1	-5.35	112.78	120.80
1	B	48	GLU	CA-C-N	5.34	129.76	120.68
1	B	48	GLU	C-N-CA	5.34	129.76	120.68
1	B	71	ARG	NH1-CZ-NH2	5.34	126.24	119.30
1	A	73	THR	CA-CB-OG1	-5.33	101.60	109.60
1	B	44	ARG	CA-CB-CG	-5.33	103.44	114.10
1	B	65	GLN	CB-CG-CD	-5.33	103.54	112.60
1	A	134	GLU	OE1-CD-OE2	5.32	135.67	122.90
1	B	132	ASP	CB-CA-C	-5.32	100.91	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	O-C-N	-5.31	117.11	123.27
1	B	83	ALA	N-CA-CB	-5.31	102.05	110.22
1	A	76	LYS	O-C-N	-5.30	116.06	122.48
1	B	116	ASP	OD1-CG-OD2	5.30	135.62	122.90
1	B	88	VAL	O-C-N	5.30	127.14	121.10
1	A	78	VAL	N-CA-CB	5.30	119.97	111.23
1	B	145	ALA	CA-C-N	-5.29	113.92	122.23
1	B	145	ALA	C-N-CA	-5.29	113.92	122.23
1	A	25	PRO	CA-C-O	5.29	127.60	119.55
1	B	130	PRO	CB-CA-C	5.29	119.41	111.68
1	A	11	ASP	CB-CA-C	5.29	120.09	111.26
1	B	24	LEU	CA-C-O	5.29	127.79	121.02
1	A	34	ASN	CA-C-N	5.29	130.78	122.11
1	A	34	ASN	C-N-CA	5.29	130.78	122.11
1	B	28	LEU	N-CA-CB	-5.29	102.35	110.12
1	B	78	VAL	CA-CB-CG2	-5.29	101.42	110.40
1	A	148	SER	N-CA-C	5.28	117.78	111.71
1	A	59	ASN	CA-C-N	5.27	130.11	123.10
1	A	59	ASN	C-N-CA	5.27	130.11	123.10
1	B	119	VAL	O-C-N	5.27	129.01	123.00
1	A	58	LYS	CG-CD-CE	-5.26	99.21	111.30
1	B	10	VAL	CA-C-O	5.26	127.43	121.28
1	A	158	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
1	B	34	ASN	CA-C-O	-5.25	112.93	119.28
1	B	101	GLU	OE1-CD-OE2	5.25	135.49	122.90
1	B	38	LYS	CD-CE-NZ	-5.23	95.16	111.90
1	A	58	LYS	CA-C-N	5.23	129.36	122.30
1	A	58	LYS	C-N-CA	5.23	129.36	122.30
1	A	121	GLY	O-C-N	5.22	128.42	123.56
1	A	82	ILE	CA-CB-CG1	-5.22	101.52	110.40
1	A	42	MET	CA-C-N	-5.22	117.10	122.27
1	A	42	MET	C-N-CA	-5.22	117.10	122.27
1	B	130	PRO	CA-C-O	-5.20	111.72	119.00
1	B	98	ARG	O-C-N	-5.19	115.37	122.33
1	A	128	TYR	CB-CG-CD1	5.18	128.57	120.80
1	A	29	ALA	CA-C-O	5.17	126.04	120.55
1	B	158	ARG	CG-CD-NE	-5.17	100.62	112.00
1	A	100	TYR	CB-CG-CD2	-5.17	113.04	120.80
1	A	146	GLN	CA-CB-CG	-5.17	103.76	114.10
1	A	22	TRP	CG-CD1-NE1	5.17	116.92	110.20
1	B	105	PRO	CA-C-N	5.17	130.75	121.66
1	B	105	PRO	C-N-CA	5.17	130.75	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	ASN	CA-C-N	-5.16	114.14	122.24
1	B	34	ASN	C-N-CA	-5.16	114.14	122.24
1	B	14	ILE	O-C-N	-5.15	112.97	121.67
1	B	22	TRP	CA-CB-CG	5.15	123.39	113.60
1	A	149	HIS	CA-C-N	5.13	128.49	120.75
1	A	149	HIS	C-N-CA	5.13	128.49	120.75
1	A	2	ILE	CA-CB-CG2	5.12	119.21	110.50
1	A	34	ASN	CA-CB-CG	-5.12	107.47	112.60
1	A	107	ALA	N-CA-C	5.11	118.27	110.20
1	B	74	TRP	CA-C-O	5.08	126.44	120.80
1	B	39	PRO	O-C-N	-5.08	116.67	123.06
1	B	133	TRP	CD2-CE3-CZ3	5.08	125.20	118.60
1	A	47	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	A	93	VAL	CA-CB-CG2	-5.06	101.79	110.40
1	A	131	ASP	CA-C-N	5.06	130.71	122.67
1	A	131	ASP	C-N-CA	5.06	130.71	122.67
1	B	87	ASP	CA-C-O	5.05	127.33	121.11
1	B	140	PHE	N-CA-CB	-5.05	102.76	110.85
1	A	30	TRP	CG-CD1-NE1	-5.05	103.63	110.20
1	B	69	ASP	CA-C-O	5.05	126.66	120.60
1	A	99	VAL	N-CA-C	-5.05	105.57	110.42
1	B	140	PHE	CZ-CE2-CD2	-5.05	110.92	120.00
1	B	57	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	44	ARG	CG-CD-NE	-5.04	100.92	112.00
1	B	143	ALA	CA-C-O	-5.03	116.22	121.55
1	A	123	THR	CA-C-N	-5.03	114.78	122.62
1	A	123	THR	C-N-CA	-5.03	114.78	122.62
1	A	3	SER	CA-CB-OG	-5.03	101.05	111.10
1	B	114	HIS	CG-CD2-NE2	5.03	112.22	107.20
1	A	108	GLN	O-C-N	-5.02	115.76	122.49
1	B	158	ARG	CA-CB-CG	-5.02	104.06	114.10
1	B	34	ASN	CA-CB-CG	-5.01	107.59	112.60
1	B	110	LEU	N-CA-CB	5.01	119.47	110.80
1	B	94	ILE	O-C-N	5.01	126.72	122.16
1	A	116	ASP	CB-CA-C	5.01	120.06	112.00
1	A	127	ASP	OD1-CG-OD2	-5.01	110.89	122.90

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	65	GLN	Peptide,Mainchain
1	A	98	ARG	Sidechain
1	B	101	GLU	Mainchain
1	B	12	ARG	Sidechain,Mainchain
1	B	29	ALA	Mainchain
1	B	33	ARG	Sidechain
1	B	41	ILE	Mainchain
1	B	44	ARG	Sidechain
1	B	45[B]	HIS	Mainchain
1	B	52	ARG	Sidechain
1	B	55	PRO	Mainchain
1	B	60	ILE	Mainchain
1	B	64[B]	SER	Mainchain
1	B	7	ALA	Mainchain
1	B	71	ARG	Sidechain
1	B	98	ARG	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	1252	0	1183	25	0
1	B	1286	0	1228	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	19	2	0
3	B	33	0	20	0	0
4	B	1	0	0	0	0
5	A	239	0	0	11	0
5	B	189	0	0	9	0
All	All	3035	0	2450	59	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 12.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:CA	1:B:57:ARG:CB	1.74	1.61
1:A:58:LYS:CD	1:A:58:LYS:CE	1.75	1.57
1:A:109:LYS:CE	1:A:109:LYS:NZ	1.70	1.52
1:B:159:ARG:N	1:B:159:ARG:CA	1.70	1.49
1:B:122[B]:ASP:C	1:B:123:THR:N	1.82	1.37
1:B:64[B]:SER:OG	1:B:65:GLN:NE2	1.86	1.06
1:A:64[B]:SER:HB3	5:A:229:HOH:O	1.60	1.01
1:B:124:HIS:HB3	5:B:342:HOH:O	1.59	0.99
1:A:51:GLY:HA3	5:B:167:HOH:O	1.70	0.89
1:B:57:ARG:CA	1:B:57:ARG:CG	2.50	0.89
1:A:58:LYS:CE	1:A:58:LYS:CG	2.52	0.88
1:B:158:ARG:C	1:B:159:ARG:CA	2.49	0.85
1:B:159:ARG:N	1:B:159:ARG:CB	2.40	0.84
1:B:57:ARG:CB	1:B:57:ARG:N	2.42	0.81
1:B:57:ARG:CB	1:B:57:ARG:C	2.56	0.77
1:A:46:THR:OG1	5:A:376:HOH:O	2.05	0.75
1:A:58:LYS:CD	1:A:58:LYS:NZ	2.54	0.71
1:B:1:MET:HE3	1:B:90:GLU:HG3	1.73	0.71
1:B:108:GLN:HG2	5:B:181:HOH:O	1.93	0.68
1:B:159:ARG:N	1:B:159:ARG:C	2.54	0.63
1:B:129:GLU:HB3	1:B:132:ASP:OD2	1.99	0.61
1:A:33:ARG:HG3	5:A:239:HOH:O	2.01	0.60
1:A:109:LYS:NZ	1:A:109:LYS:CD	2.58	0.59
1:A:67:GLY:HA2	1:A:74:TRP:CE2	2.38	0.58
1:B:45[B]:HIS:HD2	5:B:329:HOH:O	1.86	0.57
1:A:78:VAL:O	1:A:82:ILE:HD12	2.04	0.57
1:A:95:GLY:C	5:A:376:HOH:O	2.46	0.56
1:B:12:ARG:NH1	5:B:342:HOH:O	2.38	0.56
1:B:75:VAL:HG21	1:B:81:ALA:HB2	1.87	0.55
1:A:128:TYR:O	1:A:130:PRO:HD3	2.07	0.55
1:A:67:GLY:HA2	1:A:74:TRP:CD2	2.43	0.54
1:B:64[A]:SER:HB2	1:B:65:GLN:NE2	2.21	0.54
3:A:161:MTX:HG1	5:A:328:HOH:O	2.11	0.51
1:B:97:GLY:O	1:B:101:GLU:HG3	2.11	0.50
1:B:12:ARG:HB2	5:B:342:HOH:O	2.12	0.49
1:A:134:GLU:HG3	5:A:373:HOH:O	2.11	0.49
1:B:146:GLN:OE1	5:B:167:HOH:O	2.20	0.49
1:B:57:ARG:CA	1:B:57:ARG:HG3	2.42	0.48
1:A:44:ARG:O	1:A:44:ARG:HG3	2.15	0.47
1:A:27:ASP:OD2	3:A:161:MTX:N1	2.48	0.46
1:B:64[A]:SER:CB	1:B:65:GLN:HE21	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:O	1:B:48:GLU:HG3	2.16	0.46
1:B:16:MET:HE1	5:B:211:HOH:O	2.16	0.46
1:B:64[A]:SER:HB2	1:B:65:GLN:HE21	1.80	0.46
1:B:1:MET:O	1:B:90:GLU:HA	2.17	0.45
1:A:10:VAL:HG22	1:A:117:ALA:O	2.17	0.45
1:A:114:HIS:CD2	5:A:381:HOH:O	2.70	0.44
1:A:46:THR:CB	5:A:376:HOH:O	2.62	0.43
1:B:12:ARG:CZ	5:B:342:HOH:O	2.67	0.43
1:B:65:GLN:HA	1:B:66:PRO:HD3	1.79	0.43
1:A:95:GLY:CA	5:A:376:HOH:O	2.67	0.42
1:B:44:ARG:HH12	1:B:68:THR:HG23	1.84	0.42
1:B:75:VAL:HG21	1:B:81:ALA:CB	2.49	0.41
1:A:46:THR:CG2	5:A:376:HOH:O	2.69	0.41
1:A:92:MET:HE1	1:A:111:TYR:CE1	2.55	0.40
1:A:158:ARG:NH2	5:A:199:HOH:O	2.54	0.40
1:B:4:LEU:HD13	1:B:107:ALA:HB2	2.03	0.40
1:A:54:LEU:HA	1:A:55:PRO:HD3	1.96	0.40
1:B:44:ARG:HH12	1:B:68:THR:CG2	2.34	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	158/159 (99%)	146 (92%)	10 (6%)	2 (1%)	9	2
1	B	160/159 (101%)	156 (98%)	4 (2%)	0	100	100
All	All	318/318 (100%)	302 (95%)	14 (4%)	2 (1%)	21	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLY
1	A	66	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/136 (96%)	116 (89%)	14 (11%)	6	1
1	B	137/136 (101%)	128 (93%)	9 (7%)	15	4
All	All	267/272 (98%)	244 (91%)	23 (9%)	10	2

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	12	ARG
1	A	21	PRO
1	A	61	ILE
1	A	62	LEU
1	A	64[A]	SER
1	A	64[B]	SER
1	A	80	GLU
1	A	87	ASP
1	A	98	ARG
1	A	104	LEU
1	A	109	LYS
1	A	120	GLU
1	A	136	VAL
1	B	1	MET
1	B	4	LEU
1	B	52	ARG
1	B	59	ASN
1	B	61	ILE
1	B	68	THR
1	B	111	TYR
1	B	118	GLU

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Mol	Chain	Res	Type
1	B	158	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	114	HIS
1	B	23	ASN
1	B	65	GLN
1	B	124	HIS

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MTX	A	161	-	35,35,35	3.28	17 (48%)	47,49,49	4.33	25 (53%)
3	MTX	B	162	-	35,35,35	3.27	15 (42%)	47,49,49	3.91	25 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTX	A	161	-	-	2/25/25/25	0/3/3/3
3	MTX	B	162	-	-	3/25/25/25	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	162	MTX	CG-CD	10.10	1.74	1.50
3	A	161	MTX	C4A-C8A	-8.54	1.26	1.40
3	A	161	MTX	CG-CD	7.49	1.67	1.50
3	B	162	MTX	C7-C6	-6.00	1.28	1.39
3	B	162	MTX	C9-N10	5.74	1.57	1.46
3	A	161	MTX	CM-N10	5.43	1.54	1.46
3	A	161	MTX	C14-N10	5.43	1.54	1.38
3	B	162	MTX	CM-N10	5.26	1.54	1.46
3	A	161	MTX	CA-N	5.21	1.56	1.45
3	B	162	MTX	OE1-CD	4.97	1.38	1.22
3	B	162	MTX	O1-CT	4.69	1.36	1.22
3	A	161	MTX	O-C	4.60	1.34	1.23
3	A	161	MTX	C7-C6	4.52	1.47	1.39
3	B	162	MTX	CA-CT	-4.36	1.41	1.52
3	B	162	MTX	CB-CG	4.29	1.65	1.52
3	A	161	MTX	C8A-N8	4.18	1.43	1.37
3	A	161	MTX	C16-C11	-4.01	1.33	1.39
3	A	161	MTX	OE1-CD	3.93	1.35	1.22
3	B	162	MTX	C2-NA2	3.92	1.41	1.33
3	B	162	MTX	C8A-N1	3.79	1.44	1.36
3	A	161	MTX	C9-N10	3.70	1.53	1.46
3	B	162	MTX	C4A-C8A	-3.68	1.34	1.40
3	A	161	MTX	C15-C14	3.35	1.45	1.39
3	A	161	MTX	C4-NA4	-2.84	1.23	1.34
3	B	162	MTX	C16-C15	-2.78	1.34	1.38
3	A	161	MTX	C13-C14	-2.58	1.34	1.39
3	B	162	MTX	C8A-N8	2.57	1.40	1.37
3	A	161	MTX	CB-CG	2.29	1.59	1.52
3	B	162	MTX	C16-C11	2.26	1.42	1.39
3	A	161	MTX	C2-N3	-2.18	1.31	1.35
3	B	162	MTX	C7-N8	2.08	1.35	1.31
3	A	161	MTX	OE2-CD	2.01	1.37	1.30

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	161	MTX	C4A-C4-N3	-13.21	105.21	120.84
3	A	161	MTX	C2-N1-C8A	-10.00	104.71	115.48
3	A	161	MTX	N8-C8A-N1	-9.85	105.02	115.77
3	B	162	MTX	CM-N10-C14	9.03	134.54	119.59
3	B	162	MTX	C7-N8-C8A	-8.95	104.72	117.20
3	A	161	MTX	CB-CG-CD	8.63	135.52	112.49
3	B	162	MTX	C6-C7-N8	8.38	131.18	123.14
3	B	162	MTX	C4-C4A-N5	-7.34	114.67	120.33
3	B	162	MTX	O2-CT-O1	-7.27	107.59	124.08
3	A	161	MTX	C4-C4A-N5	-6.70	115.16	120.33
3	B	162	MTX	CB-CG-CD	6.46	129.72	112.49
3	B	162	MTX	C15-C16-C11	-6.46	113.90	120.80
3	B	162	MTX	O2-CT-CA	6.16	134.37	113.51
3	A	161	MTX	CG-CB-CA	-5.89	102.30	113.16
3	A	161	MTX	CT-CA-N	-5.82	97.06	110.57
3	B	162	MTX	C16-C11-C12	5.80	125.95	118.57
3	A	161	MTX	C11-C-N	-5.66	106.55	117.04
3	A	161	MTX	C4A-C8A-N1	5.35	130.03	121.74
3	B	162	MTX	OE1-CD-CG	-5.31	106.25	123.09
3	A	161	MTX	C9-N10-C14	5.24	126.52	120.17
3	B	162	MTX	CM-N10-C9	-5.10	101.83	115.11
3	B	162	MTX	C13-C14-N10	-4.67	115.08	121.59
3	A	161	MTX	OE2-CD-CG	-4.38	100.16	114.00
3	A	161	MTX	C4A-C4-NA4	4.36	126.95	120.31
3	A	161	MTX	C6-C7-N8	-4.29	119.03	123.14
3	A	161	MTX	OE1-CD-CG	4.28	136.67	123.09
3	A	161	MTX	O-C-N	4.26	130.56	122.47
3	B	162	MTX	C6-N5-C4A	-4.25	112.16	118.17
3	A	161	MTX	C13-C12-C11	4.10	125.18	120.80
3	A	161	MTX	NA4-C4-N3	3.99	127.83	117.11
3	B	162	MTX	C4A-C4-N3	-3.98	116.13	120.84
3	A	161	MTX	C2-N3-C4	3.86	127.73	116.72
3	B	162	MTX	OE2-CD-OE1	3.78	133.05	123.33
3	A	161	MTX	CB-CA-CT	-3.66	101.68	110.35
3	A	161	MTX	C15-C16-C11	-3.65	116.90	120.80
3	B	162	MTX	C13-C12-C11	-3.63	116.92	120.80
3	A	161	MTX	C12-C13-C14	-3.50	115.86	120.30
3	B	162	MTX	CG-CB-CA	-3.41	106.86	113.16
3	A	161	MTX	O2-CT-O1	-3.08	117.09	124.08
3	B	162	MTX	N8-C8A-N1	-2.88	112.62	115.77
3	B	162	MTX	OE2-CD-CG	-2.78	105.22	114.00
3	A	161	MTX	NA2-C2-N1	-2.75	113.49	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	162	MTX	C9-N10-C14	2.62	123.35	120.17
3	B	162	MTX	C4A-C4-NA4	2.58	124.24	120.31
3	B	162	MTX	C7-C6-N5	2.57	122.54	120.87
3	A	161	MTX	C16-C15-C14	2.39	123.33	120.30
3	B	162	MTX	CB-CA-CT	-2.28	104.95	110.35
3	B	162	MTX	N1-C2-N3	-2.14	124.49	127.21
3	B	162	MTX	C12-C11-C	-2.10	113.80	120.60
3	A	161	MTX	CB-CA-N	2.08	115.03	110.91

There are no chirality outliers.

All (5) torsion outliers are listed below:

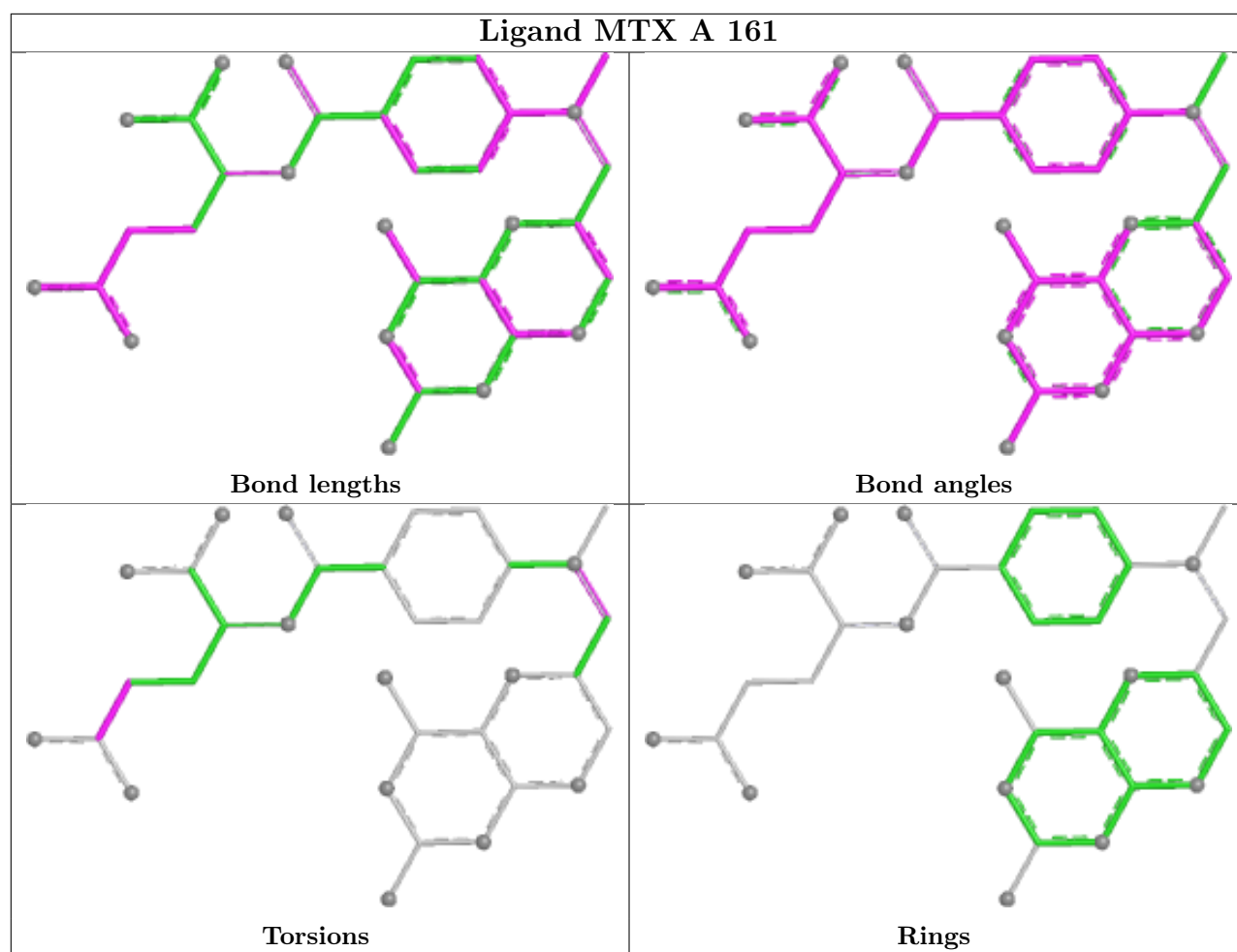
Mol	Chain	Res	Type	Atoms
3	A	161	MTX	C6-C9-N10-CM
3	B	162	MTX	OE1-CD-CG-CB
3	B	162	MTX	C6-C9-N10-CM
3	A	161	MTX	OE2-CD-CG-CB
3	B	162	MTX	C6-C9-N10-C14

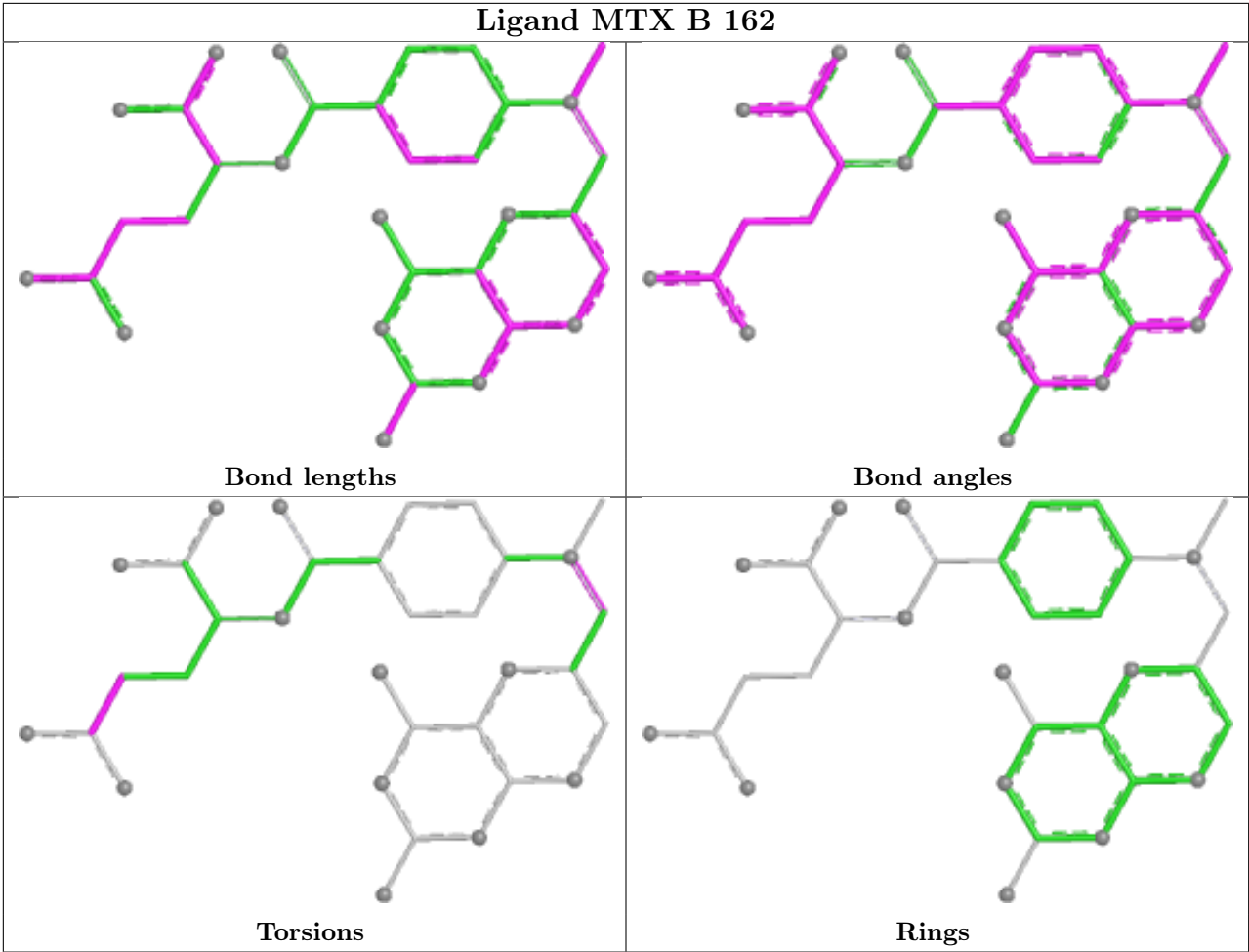
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	161	MTX	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	12
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	122[B]:ASP	C	123:THR	N	1.82
1	B	44:ARG	C	45[B]:HIS	N	1.65
1	A	30:TRP	C	31:PHE	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	34:ASN	C	35:THR	N	1.20
1	B	154:LYS	C	155:ILE	N	1.20
1	A	127:ASP	C	128:TYR	N	1.19
1	A	143:ALA	C	144:ASP	N	1.19
1	A	151:TYR	C	152:CYS	N	1.19
1	B	151:TYR	C	152:CYS	N	1.19
1	B	59:ASN	C	60:ILE	N	1.18
1	B	153:PHE	C	154:LYS	N	1.18
1	A	44:ARG	C	45:HIS	N	1.17
1	B	64[B]:SER	C	65:GLN	N	1.15
1	B	114:HIS	C	115:ILE	N	1.15
1	A	111:TYR	C	112:LEU	N	1.13
1	B	110:LEU	C	111:TYR	N	1.12
1	A	109:LYS	C	110:LEU	N	1.11
1	B	63:SER	C	64[B]:SER	N	1.02
1	B	121:GLY	C	122[B]:ASP	N	0.97

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.