



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:46 PM GMT

PDB ID : 4DFR
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

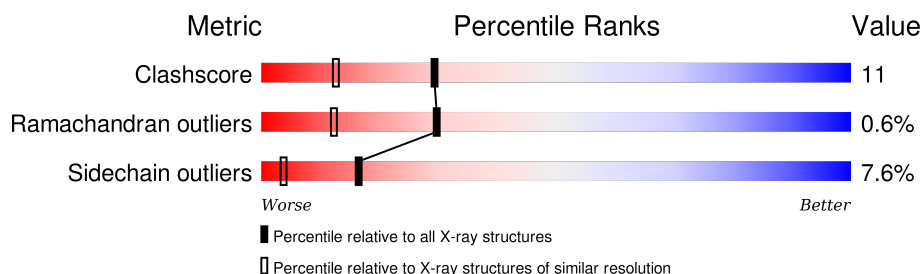
1 Overall quality at a glance

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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	 13% 65% 18% •
1	B	159	 8% 70% 16% 6%

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

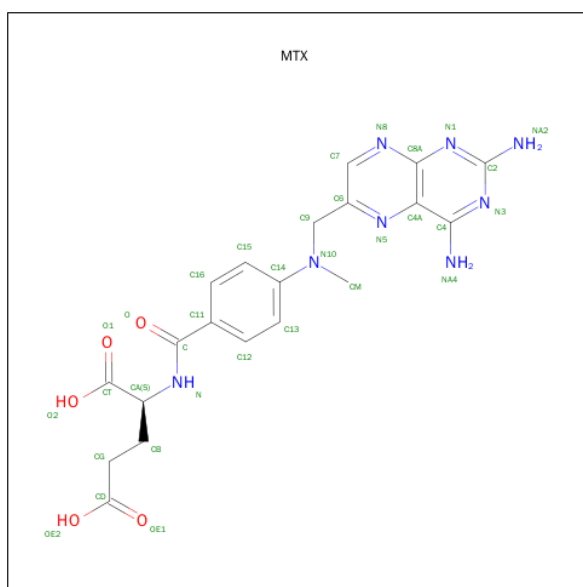
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 33	C 20	N 8	O 5	0	0
4	B	1	Total 33	C 20	N 8	O 5	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

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 will therefore be 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: MTX, CA, 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	3.24	144/1285 (11.2%)	4.42	311/1747 (17.8%)
1	B	3.44	163/1321 (12.3%)	4.72	340/1795 (18.9%)
All	All	3.34	307/2606 (11.8%)	4.58	651/3542 (18.4%)

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 (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	SER	CB-OG	-20.55	1.15	1.42
1	B	57	ARG	CZ-NH1	16.57	1.54	1.33
1	B	100	TYR	CG-CD2	15.22	1.58	1.39
1	A	48	GLU	CD-OE2	14.75	1.41	1.25
1	B	118	GLU	CD-OE2	14.05	1.41	1.25
1	B	33	ARG	NE-CZ	13.07	1.50	1.33
1	A	33	ARG	CZ-NH2	13.06	1.50	1.33
1	B	17	GLU	CD-OE2	12.58	1.39	1.25
1	A	22	TRP	CD2-CE2	-12.33	1.26	1.41
1	A	64[A]	SER	CB-OG	12.03	1.57	1.42
1	A	64[B]	SER	CB-OG	12.03	1.57	1.42
1	B	159	ARG	N-CA	11.91	1.70	1.46
1	B	55	PRO	C-O	11.84	1.47	1.23
1	B	111	TYR	CG-CD1	-11.16	1.24	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	GLU	CD-OE2	10.64	1.37	1.25
1	A	111	TYR	C-O	10.56	1.43	1.23
1	A	43	GLY	C-O	10.54	1.40	1.23
1	A	120	GLU	CD-OE2	10.47	1.37	1.25
1	B	74	TRP	CD1-NE1	-10.34	1.20	1.38
1	B	22	TRP	CZ3-CH2	-10.14	1.23	1.40
1	B	101	GLU	CG-CD	10.10	1.67	1.51
1	B	139	GLU	CD-OE2	9.98	1.36	1.25
1	B	93	VAL	C-O	9.80	1.42	1.23
1	A	48	GLU	CB-CG	-9.76	1.33	1.52
1	A	109	LYS	C-N	-9.75	1.11	1.34
1	A	58	LYS	CD-CE	9.71	1.75	1.51
1	B	45[A]	HIS	CB-CG	9.67	1.67	1.50
1	B	45[B]	HIS	CB-CG	9.67	1.67	1.50
1	B	55	PRO	CA-C	-9.64	1.33	1.52
1	B	57	ARG	CA-CB	9.46	1.74	1.53
1	A	22	TRP	CZ3-CH2	-9.38	1.25	1.40
1	B	38	LYS	CD-CE	9.27	1.74	1.51
1	A	30	TRP	CD2-CE2	-9.26	1.30	1.41
1	B	12	ARG	CZ-NH1	9.26	1.45	1.33
1	B	110	LEU	C-N	-9.22	1.12	1.34
1	B	118	GLU	CD-OE1	9.20	1.35	1.25
1	B	139	GLU	CG-CD	-9.19	1.38	1.51
1	A	159	ARG	C-O	9.15	1.40	1.23
1	A	111	TYR	C-N	-8.95	1.13	1.34
1	A	52	ARG	CZ-NH1	8.94	1.44	1.33
1	A	57	ARG	CZ-NH2	8.90	1.44	1.33
1	B	60	ILE	C-O	8.82	1.40	1.23
1	B	101	GLU	CA-CB	-8.77	1.34	1.53
1	B	44	ARG	CA-CB	8.72	1.73	1.53
1	B	17	GLU	CB-CG	-8.64	1.35	1.52
1	A	109	LYS	CE-NZ	8.59	1.70	1.49
1	B	97	GLY	N-CA	8.59	1.58	1.46
1	B	159	ARG	NE-CZ	8.59	1.44	1.33
1	B	123	THR	CB-OG1	8.55	1.60	1.43
1	B	149	HIS	CB-CG	8.53	1.65	1.50
1	A	51	GLY	N-CA	-8.52	1.33	1.46
1	A	71	ARG	NE-CZ	-8.45	1.22	1.33
1	B	18	ASN	CB-CG	8.39	1.70	1.51
1	A	33	ARG	CZ-NH1	8.36	1.44	1.33
1	A	78	VAL	C-O	8.31	1.39	1.23
1	A	47	TRP	CD2-CE3	-8.25	1.27	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	VAL	CB-CG2	8.17	1.70	1.52
1	B	44	ARG	NE-CZ	8.17	1.43	1.33
1	B	74	TRP	CD2-CE2	-8.16	1.31	1.41
1	B	114	HIS	C-N	-8.12	1.15	1.34
1	B	80	GLU	CD-OE1	8.07	1.34	1.25
1	A	77	SER	CA-CB	8.00	1.65	1.52
1	A	109	LYS	CB-CG	-8.00	1.30	1.52
1	A	133	TRP	NE1-CE2	7.97	1.48	1.37
1	B	80	GLU	CD-OE2	7.95	1.34	1.25
1	A	143	ALA	C-O	7.93	1.38	1.23
1	A	115	ILE	CA-CB	7.93	1.73	1.54
1	A	100	TYR	C-O	-7.92	1.08	1.23
1	B	100	TYR	CE1-CZ	-7.89	1.28	1.38
1	A	113	THR	CB-OG1	-7.86	1.27	1.43
1	B	134	GLU	CB-CG	7.83	1.67	1.52
1	B	114	HIS	CG-CD2	-7.79	1.22	1.35
1	A	103	PHE	CA-C	-7.75	1.32	1.52
1	B	151	TYR	CZ-OH	-7.74	1.24	1.37
1	B	22	TRP	CE3-CZ3	7.74	1.51	1.38
1	A	133	TRP	CA-CB	7.71	1.71	1.53
1	B	49	SER	CB-OG	7.71	1.52	1.42
1	A	151	TYR	CD1-CE1	7.70	1.50	1.39
1	B	72	VAL	C-O	7.67	1.38	1.23
1	A	3	SER	CB-OG	7.67	1.52	1.42
1	A	44	ARG	CD-NE	7.63	1.59	1.46
1	B	1	MET	CA-C	7.58	1.72	1.52
1	B	6	ALA	CA-CB	7.57	1.68	1.52
1	B	111	TYR	CA-C	-7.54	1.33	1.52
1	A	157	GLU	CD-OE2	7.53	1.33	1.25
1	A	65	GLN	C-O	7.52	1.37	1.23
1	A	6	ALA	CA-CB	7.51	1.68	1.52
1	A	90	GLU	CA-CB	-7.50	1.37	1.53
1	B	43	GLY	CA-C	-7.49	1.39	1.51
1	A	146	GLN	CD-OE1	7.47	1.40	1.24
1	B	116	ASP	C-O	7.44	1.37	1.23
1	B	111	TYR	CD2-CE2	7.43	1.50	1.39
1	B	124	HIS	C-O	7.42	1.37	1.23
1	B	31	PHE	CE2-CZ	7.40	1.51	1.37
1	A	131	ASP	C-O	7.37	1.37	1.23
1	A	9	ALA	C-O	7.37	1.37	1.23
1	A	1	MET	CA-CB	-7.36	1.37	1.53
1	A	93	VAL	C-O	7.30	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLU	CD-OE2	-7.26	1.17	1.25
1	A	56	GLY	N-CA	-7.25	1.35	1.46
1	A	105	PRO	N-CD	7.21	1.57	1.47
1	A	123	THR	C-O	-7.17	1.09	1.23
1	A	49	SER	CB-OG	7.17	1.51	1.42
1	B	2	ILE	CB-CG1	7.16	1.74	1.54
1	B	111	TYR	C-O	7.11	1.36	1.23
1	A	126	PRO	N-CA	7.08	1.59	1.47
1	B	159	ARG	CA-CB	-7.07	1.38	1.53
1	A	98	ARG	CD-NE	7.06	1.58	1.46
1	A	90	GLU	CG-CD	-7.05	1.41	1.51
1	A	134	GLU	CD-OE1	7.04	1.33	1.25
1	A	44	ARG	C-N	-7.04	1.17	1.34
1	B	47	TRP	CE2-CZ2	7.02	1.51	1.39
1	B	90	GLU	CD-OE1	-7.02	1.18	1.25
1	B	12	ARG	NE-CZ	-7.00	1.24	1.33
1	B	154	LYS	CD-CE	6.99	1.68	1.51
1	A	55	PRO	C-N	-6.99	1.20	1.33
1	A	53	PRO	C-O	-6.95	1.09	1.23
1	A	152	CYS	CA-C	-6.95	1.34	1.52
1	B	21	PRO	N-CD	6.93	1.57	1.47
1	B	59	ASN	C-O	6.87	1.36	1.23
1	A	120	GLU	CD-OE1	6.86	1.33	1.25
1	B	68	THR	CB-OG1	6.86	1.56	1.43
1	B	33	ARG	CG-CD	6.86	1.69	1.51
1	B	97	GLY	CA-C	-6.82	1.41	1.51
1	B	116	ASP	CB-CG	6.82	1.66	1.51
1	B	56	GLY	N-CA	-6.81	1.35	1.46
1	B	153	PHE	C-N	-6.81	1.18	1.34
1	B	114	HIS	CG-ND1	6.81	1.53	1.38
1	B	54	LEU	CA-CB	6.80	1.69	1.53
1	B	59	ASN	C-N	-6.69	1.18	1.34
1	B	141	HIS	CD2-NE2	6.68	1.55	1.42
1	B	52	ARG	NE-CZ	6.68	1.41	1.33
1	A	6	ALA	C-O	6.68	1.36	1.23
1	A	44	ARG	CG-CD	-6.66	1.35	1.51
1	A	128	TYR	CG-CD1	-6.66	1.30	1.39
1	B	55	PRO	C-N	-6.63	1.21	1.33
1	B	39	PRO	N-CD	-6.63	1.38	1.47
1	B	154	LYS	C-O	6.62	1.35	1.23
1	B	3	SER	CB-OG	-6.60	1.33	1.42
1	A	127	ASP	CG-OD2	6.58	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	GLN	N-CA	6.58	1.59	1.46
1	B	151	TYR	C-N	-6.54	1.19	1.34
1	A	12	ARG	CZ-NH2	6.53	1.41	1.33
1	A	125	PHE	CG-CD1	6.53	1.48	1.38
1	A	143	ALA	C-N	-6.52	1.19	1.34
1	B	10	VAL	CB-CG2	6.49	1.66	1.52
1	A	155	ILE	N-CA	-6.48	1.33	1.46
1	B	42	MET	C-O	-6.46	1.11	1.23
1	B	139	GLU	CD-OE1	-6.45	1.18	1.25
1	A	12	ARG	CZ-NH1	6.45	1.41	1.33
1	A	74	TRP	CB-CG	-6.44	1.38	1.50
1	A	116	ASP	CA-C	-6.44	1.36	1.52
1	B	57	ARG	NE-CZ	-6.40	1.24	1.33
1	B	102	GLN	CA-C	-6.40	1.36	1.52
1	A	135	SER	CB-OG	-6.36	1.33	1.42
1	B	135	SER	CA-CB	6.33	1.62	1.52
1	A	57	ARG	CD-NE	-6.31	1.35	1.46
1	B	93	VAL	CA-C	-6.31	1.36	1.52
1	B	6	ALA	C-O	6.25	1.35	1.23
1	B	131	ASP	CA-CB	6.24	1.67	1.53
1	A	151	TYR	CD2-CE2	-6.22	1.30	1.39
1	A	151	TYR	C-N	-6.20	1.19	1.34
1	B	158	ARG	CA-CB	6.20	1.67	1.53
1	A	127	ASP	C-N	-6.18	1.19	1.34
1	B	111	TYR	N-CA	6.18	1.58	1.46
1	B	33	ARG	C-N	6.14	1.48	1.34
1	B	18	ASN	C-O	-6.14	1.11	1.23
1	A	132	ASP	C-O	-6.12	1.11	1.23
1	A	158	ARG	CD-NE	6.08	1.56	1.46
1	A	90	GLU	CD-OE1	-6.04	1.19	1.25
1	B	34	ASN	C-N	-6.04	1.20	1.34
1	A	142	ASP	CB-CG	6.02	1.64	1.51
1	B	72	VAL	CA-CB	6.02	1.67	1.54
1	A	30	TRP	C-N	-6.02	1.20	1.34
1	B	154	LYS	C-N	-6.01	1.20	1.34
1	B	17	GLU	CD-OE1	6.01	1.32	1.25
1	B	12	ARG	CZ-NH2	6.01	1.40	1.33
1	A	47	TRP	CG-CD1	-5.98	1.28	1.36
1	A	25	PRO	CA-CB	-5.97	1.41	1.53
1	B	122[A]	ASP	CG-OD1	5.97	1.39	1.25
1	B	122[B]	ASP	CG-OD1	5.97	1.39	1.25
1	A	98	ARG	C-O	-5.96	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	TRP	CD2-CE3	5.94	1.49	1.40
1	A	43	GLY	N-CA	-5.94	1.37	1.46
1	A	158	ARG	CZ-NH2	5.93	1.40	1.33
1	B	17	GLU	CG-CD	5.90	1.60	1.51
1	B	159	ARG	C-OXT	5.90	1.34	1.23
1	B	150	SER	CB-OG	-5.90	1.34	1.42
1	A	33	ARG	N-CA	5.89	1.58	1.46
1	B	45[A]	HIS	CA-CB	5.89	1.67	1.53
1	B	45[B]	HIS	CA-CB	5.89	1.67	1.53
1	A	80	GLU	CD-OE2	5.87	1.32	1.25
1	B	45[A]	HIS	CG-CD2	5.83	1.45	1.35
1	B	45[B]	HIS	CG-CD2	5.83	1.45	1.35
1	A	73	THR	C-O	-5.83	1.12	1.23
1	A	72	VAL	C-N	-5.80	1.20	1.34
1	A	103	PHE	CE1-CZ	-5.80	1.26	1.37
1	A	101	GLU	CD-OE1	5.79	1.32	1.25
1	B	20	MET	CA-CB	-5.79	1.41	1.53
1	A	18	ASN	C-O	5.79	1.34	1.23
1	A	44	ARG	N-CA	-5.78	1.34	1.46
1	B	51	GLY	CA-C	-5.78	1.42	1.51
1	A	103	PHE	CG-CD1	5.77	1.47	1.38
1	A	22	TRP	CD1-NE1	5.77	1.47	1.38
1	A	17	GLU	CA-C	5.77	1.68	1.52
1	A	102	GLN	CD-OE1	5.76	1.36	1.24
1	B	93	VAL	C-N	-5.75	1.20	1.34
1	A	154	LYS	CE-NZ	5.75	1.63	1.49
1	A	139	GLU	C-O	5.74	1.34	1.23
1	B	133	TRP	C-N	-5.73	1.20	1.34
1	B	158	ARG	CG-CD	5.71	1.66	1.51
1	B	7	ALA	C-O	5.71	1.34	1.23
1	B	104	LEU	N-CA	5.71	1.57	1.46
1	B	128	TYR	CZ-OH	5.70	1.47	1.37
1	A	26	ALA	CA-CB	5.69	1.64	1.52
1	A	156	LEU	CA-C	-5.67	1.38	1.52
1	B	75	VAL	CB-CG2	5.67	1.64	1.52
1	A	85	CYS	N-CA	-5.66	1.35	1.46
1	B	96	GLY	C-N	5.66	1.43	1.33
1	A	98	ARG	CZ-NH1	5.65	1.40	1.33
1	B	43	GLY	C-O	5.65	1.32	1.23
1	B	120	GLU	CD-OE1	5.64	1.31	1.25
1	B	159	ARG	CZ-NH1	-5.61	1.25	1.33
1	B	33	ARG	CD-NE	5.61	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	ALA	C-O	5.60	1.33	1.23
1	A	138	SER	CB-OG	-5.59	1.34	1.42
1	B	116	ASP	N-CA	5.59	1.57	1.46
1	A	98	ARG	CZ-NH2	5.58	1.40	1.33
1	A	98	ARG	NE-CZ	5.57	1.40	1.33
1	B	59	ASN	CB-CG	-5.55	1.38	1.51
1	B	93	VAL	CB-CG2	-5.54	1.41	1.52
1	A	22	TRP	CB-CG	-5.52	1.40	1.50
1	B	5	ILE	CB-CG1	5.52	1.69	1.54
1	A	88	VAL	CA-CB	5.51	1.66	1.54
1	A	118	GLU	CD-OE2	5.50	1.31	1.25
1	A	106	LYS	CG-CD	5.49	1.71	1.52
1	A	124	HIS	CE1-NE2	5.48	1.45	1.32
1	A	151	TYR	CA-C	-5.47	1.38	1.52
1	B	153	PHE	CD2-CE2	5.47	1.50	1.39
1	A	107	ALA	N-CA	-5.47	1.35	1.46
1	A	38	LYS	CD-CE	-5.47	1.37	1.51
1	A	149	HIS	CG-CD2	-5.44	1.26	1.35
1	B	102	GLN	CD-OE1	5.44	1.35	1.24
1	B	96	GLY	C-O	-5.44	1.15	1.23
1	B	10	VAL	CB-CG1	5.43	1.64	1.52
1	B	85	CYS	C-O	5.41	1.33	1.23
1	A	11	ASP	CA-C	-5.41	1.38	1.52
1	A	30	TRP	CE3-CZ3	5.40	1.47	1.38
1	B	152	CYS	C-N	-5.39	1.21	1.34
1	B	129	GLU	CB-CG	5.39	1.62	1.52
1	B	100	TYR	CB-CG	5.38	1.59	1.51
1	A	90	GLU	CD-OE2	5.37	1.31	1.25
1	B	140	PHE	C-O	-5.36	1.13	1.23
1	A	14	ILE	N-CA	-5.36	1.35	1.46
1	B	91	ILE	CB-CG1	5.35	1.69	1.54
1	B	71	ARG	NE-CZ	5.35	1.40	1.33
1	B	120	GLU	CD-OE2	5.35	1.31	1.25
1	B	153	PHE	CG-CD1	5.34	1.46	1.38
1	A	159	ARG	C-OXT	5.33	1.33	1.23
1	B	136	VAL	N-CA	-5.33	1.35	1.46
1	B	40	VAL	C-O	5.32	1.33	1.23
1	B	90	GLU	CD-OE2	-5.32	1.19	1.25
1	B	120	GLU	CB-CG	-5.32	1.42	1.52
1	B	20	MET	C-N	5.31	1.44	1.34
1	B	122[A]	ASP	CA-C	-5.31	1.39	1.52
1	B	122[B]	ASP	CA-C	-5.31	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	MET	N-CA	5.30	1.56	1.46
1	A	143	ALA	CA-CB	5.30	1.63	1.52
1	B	136	VAL	CB-CG1	5.30	1.64	1.52
1	B	157	GLU	CD-OE1	-5.30	1.19	1.25
1	A	13	VAL	CB-CG2	5.29	1.64	1.52
1	A	95	GLY	C-N	-5.28	1.23	1.33
1	B	101	GLU	CB-CG	-5.27	1.42	1.52
1	A	31	PHE	CE1-CZ	5.24	1.47	1.37
1	A	48	GLU	CA-C	-5.24	1.39	1.52
1	A	30	TRP	CZ2-CH2	-5.24	1.27	1.37
1	A	42	MET	C-N	5.23	1.42	1.33
1	A	71	ARG	CZ-NH2	5.21	1.39	1.33
1	A	5	ILE	C-N	-5.20	1.22	1.34
1	B	76	LYS	CA-CB	5.20	1.65	1.53
1	B	111	TYR	CG-CD2	-5.19	1.32	1.39
1	A	110	LEU	CG-CD1	5.19	1.71	1.51
1	A	146	GLN	CA-C	-5.18	1.39	1.52
1	B	30	TRP	CD1-NE1	-5.17	1.29	1.38
1	B	44	ARG	CB-CG	5.17	1.66	1.52
1	A	1	MET	C-O	-5.16	1.13	1.23
1	A	86	GLY	N-CA	5.13	1.53	1.46
1	B	57	ARG	CZ-NH2	-5.13	1.26	1.33
1	B	53	PRO	CG-CD	5.12	1.67	1.50
1	B	121	GLY	C-N	-5.11	1.22	1.34
1	A	10	VAL	N-CA	5.11	1.56	1.46
1	B	52	ARG	CZ-NH2	5.10	1.39	1.33
1	A	152	CYS	C-O	5.10	1.33	1.23
1	B	15	GLY	C-N	-5.10	1.22	1.34
1	A	19	ALA	N-CA	5.09	1.56	1.46
1	A	112	LEU	CA-C	-5.08	1.39	1.52
1	B	121	GLY	C-O	-5.07	1.15	1.23
1	B	20	MET	CA-C	-5.07	1.39	1.52
1	B	154	LYS	CE-NZ	5.06	1.61	1.49
1	A	51	GLY	C-N	-5.06	1.22	1.34
1	B	153	PHE	CB-CG	-5.05	1.42	1.51
1	A	107	ALA	CA-CB	5.04	1.63	1.52
1	B	48	GLU	CA-C	-5.04	1.39	1.52
1	A	10	VAL	C-O	5.04	1.32	1.23
1	B	157	GLU	CG-CD	5.03	1.59	1.51
1	B	103	PHE	CG-CD1	5.02	1.46	1.38
1	A	47	TRP	NE1-CE2	-5.01	1.31	1.37

All (651) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ASP	CB-CG-OD2	-39.34	82.89	118.30
1	B	37	ASP	CB-CG-OD2	-35.23	86.59	118.30
1	A	57	ARG	NE-CZ-NH1	33.75	137.17	120.30
1	A	98	ARG	NE-CZ-NH1	31.98	136.29	120.30
1	B	71	ARG	NE-CZ-NH2	-30.39	105.11	120.30
1	B	100	TYR	CB-CG-CD2	-29.24	103.46	121.00
1	A	98	ARG	NE-CZ-NH2	-28.79	105.91	120.30
1	B	159	ARG	NE-CZ-NH2	-26.19	107.20	120.30
1	B	37	ASP	CB-CG-OD1	25.62	141.36	118.30
1	B	52	ARG	NE-CZ-NH1	25.52	133.06	120.30
1	A	116	ASP	CB-CG-OD1	25.25	141.02	118.30
1	B	158	ARG	CD-NE-CZ	24.45	157.83	123.60
1	A	57	ARG	NE-CZ-NH2	-24.44	108.08	120.30
1	A	127	ASP	CB-CG-OD1	23.54	139.49	118.30
1	B	69	ASP	CB-CG-OD1	23.53	139.47	118.30
1	A	44	ARG	NE-CZ-NH1	23.11	131.85	120.30
1	A	158	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	A	71	ARG	NE-CZ-NH2	22.11	131.35	120.30
1	B	52	ARG	CD-NE-CZ	21.95	154.32	123.60
1	B	17	GLU	OE1-CD-OE2	20.68	148.12	123.30
1	A	69	ASP	CB-CG-OD2	-19.42	100.82	118.30
1	A	16	MET	CG-SD-CE	19.05	130.68	100.20
1	B	69	ASP	CB-CG-OD2	-18.49	101.66	118.30
1	A	108	GLN	CA-CB-CG	18.25	153.56	113.40
1	B	44	ARG	NE-CZ-NH2	-18.00	111.30	120.30
1	A	79	ASP	CB-CG-OD1	17.98	134.49	118.30
1	A	11	ASP	CB-CG-OD1	17.67	134.20	118.30
1	B	55	PRO	CA-C-N	17.64	151.49	116.20
1	B	111	TYR	CB-CG-CD2	-17.46	110.52	121.00
1	B	33	ARG	NE-CZ-NH1	17.44	129.02	120.30
1	B	12	ARG	CD-NE-CZ	17.09	147.53	123.60
1	B	118	GLU	OE1-CD-OE2	-16.98	102.93	123.30
1	B	27	ASP	CB-CG-OD1	16.85	133.46	118.30
1	A	12	ARG	NE-CZ-NH2	16.80	128.70	120.30
1	A	111	TYR	CB-CG-CD2	-16.66	111.01	121.00
1	A	22	TRP	CH2-CZ2-CE2	-16.54	100.86	117.40
1	A	52	ARG	CB-CG-CD	16.43	154.31	111.60
1	B	87	ASP	CB-CG-OD1	16.21	132.89	118.30
1	B	71	ARG	NE-CZ-NH1	15.90	128.25	120.30
1	B	156	LEU	CB-CG-CD2	15.82	137.89	111.00
1	B	73	THR	CA-CB-CG2	15.48	134.07	112.40
1	B	52	ARG	CG-CD-NE	15.44	144.22	111.80
1	A	142	ASP	CB-CG-OD2	-15.33	104.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	O-C-N	15.03	146.75	122.70
1	A	22	TRP	NE1-CE2-CZ2	-14.98	113.92	130.40
1	B	52	ARG	CB-CG-CD	14.62	149.61	111.60
1	A	100	TYR	CG-CD1-CE1	-14.62	109.61	121.30
1	B	74	TRP	CE3-CZ3-CH2	-14.56	105.19	121.20
1	B	116	ASP	CB-CG-OD2	-14.56	105.20	118.30
1	A	111	TYR	CG-CD1-CE1	-14.23	109.92	121.30
1	B	27	ASP	CB-CG-OD2	-14.07	105.64	118.30
1	B	100	TYR	CB-CG-CD1	14.06	129.44	121.00
1	B	100	TYR	CG-CD1-CE1	-13.82	110.25	121.30
1	B	128	TYR	CB-CG-CD1	-13.70	112.78	121.00
1	A	31	PHE	CB-CG-CD2	-13.65	111.25	120.80
1	B	98	ARG	NE-CZ-NH2	13.51	127.05	120.30
1	B	158	ARG	NE-CZ-NH2	13.40	127.00	120.30
1	B	78	VAL	CA-CB-CG1	13.33	130.90	110.90
1	B	44	ARG	NE-CZ-NH1	13.31	126.96	120.30
1	A	135	SER	N-CA-CB	13.29	130.43	110.50
1	A	100	TYR	CB-CG-CD2	-13.26	113.04	121.00
1	A	109	LYS	CA-CB-CG	12.92	141.83	113.40
1	B	120	GLU	CB-CG-CD	12.89	149.00	114.20
1	A	8	LEU	CB-CG-CD2	12.63	132.47	111.00
1	A	128	TYR	CB-CG-CD1	12.62	128.57	121.00
1	B	79	ASP	CB-CG-OD1	12.56	129.60	118.30
1	A	132	ASP	CB-CG-OD2	-12.47	107.08	118.30
1	B	55	PRO	O-C-N	-12.46	102.01	123.20
1	B	111	TYR	O-C-N	-12.28	103.05	122.70
1	B	80	GLU	OE1-CD-OE2	12.09	137.81	123.30
1	B	122[A]	ASP	CB-CG-OD2	-12.05	107.45	118.30
1	B	122[B]	ASP	CB-CG-OD2	-12.05	107.45	118.30
1	A	22	TRP	CD1-NE1-CE2	-11.69	98.48	109.00
1	A	78	VAL	CA-CB-CG1	11.69	128.44	110.90
1	A	48	GLU	OE1-CD-OE2	11.63	137.26	123.30
1	A	73	THR	CA-CB-CG2	11.62	128.68	112.40
1	B	101	GLU	CA-CB-CG	11.57	138.85	113.40
1	B	135	SER	O-C-N	-11.51	104.29	122.70
1	B	118	GLU	CG-CD-OE2	11.49	141.28	118.30
1	B	18	ASN	OD1-CG-ND2	11.44	148.20	121.90
1	A	71	ARG	CG-CD-NE	11.43	135.81	111.80
1	A	109	LYS	CB-CG-CD	11.37	141.16	111.60
1	B	10	VAL	CG1-CB-CG2	-11.35	92.74	110.90
1	A	87	ASP	CB-CG-OD1	-11.27	108.16	118.30
1	B	140	PHE	CB-CG-CD1	11.24	128.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLY	C-N-CA	11.21	145.85	122.30
1	A	22	TRP	CD1-CG-CD2	-11.15	97.38	106.30
1	B	23	ASN	OD1-CG-ND2	-11.09	96.39	121.90
1	B	11	ASP	CB-CG-OD1	10.97	128.17	118.30
1	B	87	ASP	OD1-CG-OD2	10.97	144.14	123.30
1	B	101	GLU	O-C-N	-10.95	105.18	122.70
1	A	65	GLN	CB-CA-C	10.95	132.30	110.40
1	B	74	TRP	CZ3-CH2-CZ2	10.91	134.70	121.60
1	A	55	PRO	CA-C-N	10.88	137.96	116.20
1	B	142	ASP	CB-CG-OD2	-10.83	108.56	118.30
1	B	158	ARG	O-C-N	10.78	139.95	122.70
1	B	11	ASP	CB-CG-OD2	-10.75	108.62	118.30
1	A	44	ARG	CB-CG-CD	10.75	139.54	111.60
1	B	154	LYS	CG-CD-CE	-10.74	79.69	111.90
1	B	119	VAL	CA-CB-CG1	-10.66	94.91	110.90
1	B	4	LEU	CB-CG-CD1	10.57	128.98	111.00
1	B	111	TYR	CB-CG-CD1	10.54	127.33	121.00
1	A	116	ASP	CB-CG-OD2	-10.50	108.85	118.30
1	A	22	TRP	CE2-CD2-CG	10.49	115.69	107.30
1	B	50	ILE	O-C-N	10.42	140.92	123.20
1	A	48	GLU	CG-CD-OE2	-10.38	97.53	118.30
1	A	10	VAL	CG1-CB-CG2	-10.37	94.31	110.90
1	A	134	GLU	OE1-CD-OE2	10.31	135.67	123.30
1	B	103	PHE	CB-CG-CD1	-10.30	113.59	120.80
1	B	93	VAL	O-C-N	-10.28	106.25	122.70
1	A	71	ARG	CD-NE-CZ	10.25	137.96	123.60
1	B	36	LEU	CB-CG-CD1	10.25	128.42	111.00
1	A	71	ARG	NH1-CZ-NH2	-10.23	108.15	119.40
1	A	22	TRP	CD2-CE2-CZ2	10.22	134.56	122.30
1	A	104	LEU	CA-CB-CG	10.21	138.79	115.30
1	B	101	GLU	OE1-CD-OE2	10.16	135.49	123.30
1	A	120	GLU	CA-CB-CG	10.15	135.74	113.40
1	A	144	ASP	CB-CG-OD2	-10.15	109.17	118.30
1	A	151	TYR	CD1-CE1-CZ	-10.09	110.72	119.80
1	A	128	TYR	CG-CD1-CE1	9.98	129.29	121.30
1	B	132	ASP	CB-CG-OD2	-9.95	109.34	118.30
1	B	127	ASP	CB-CG-OD1	9.94	127.25	118.30
1	B	93	VAL	CA-C-N	9.94	139.06	117.20
1	B	12	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	59	ASN	CA-C-N	9.92	139.02	117.20
1	B	23	ASN	O-C-N	9.91	138.56	122.70
1	A	79	ASP	O-C-N	9.85	138.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ALA	C-N-CA	9.85	146.34	121.70
1	A	158	ARG	O-C-N	9.80	138.39	122.70
1	A	4	LEU	CB-CG-CD1	9.79	127.65	111.00
1	A	111	TYR	CA-C-N	9.79	138.73	117.20
1	A	31	PHE	CG-CD2-CE2	-9.75	110.08	120.80
1	A	127	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	B	1	MET	CA-CB-CG	9.72	129.83	113.30
1	A	139	GLU	CG-CD-OE1	9.71	137.72	118.30
1	A	136	VAL	CA-CB-CG1	9.67	125.41	110.90
1	B	23	ASN	CB-CG-OD1	9.62	140.84	121.60
1	B	6	ALA	O-C-N	-9.60	107.34	122.70
1	B	104	LEU	C-N-CD	9.59	148.54	128.40
1	B	158	ARG	NH1-CZ-NH2	-9.59	108.85	119.40
1	A	22	TRP	CG-CD2-CE3	-9.58	125.28	133.90
1	A	1	MET	CG-SD-CE	9.53	115.45	100.20
1	B	98	ARG	NH1-CZ-NH2	-9.52	108.93	119.40
1	B	52	ARG	NH1-CZ-NH2	-9.51	108.94	119.40
1	B	100	TYR	CZ-CE2-CD2	-9.51	111.24	119.80
1	A	6	ALA	O-C-N	-9.45	107.58	122.70
1	A	70	ASP	CB-CG-OD2	9.44	126.80	118.30
1	B	81	ALA	CA-C-O	-9.31	100.54	120.10
1	B	140	PHE	CG-CD2-CE2	9.28	131.01	120.80
1	B	30	TRP	CD1-NE1-CE2	9.25	117.32	109.00
1	B	38	LYS	O-C-N	9.23	138.65	121.10
1	B	111	TYR	CA-C-O	9.16	139.33	120.10
1	B	153	PHE	CB-CG-CD1	9.10	127.17	120.80
1	A	44	ARG	CD-NE-CZ	-9.10	110.86	123.60
1	B	103	PHE	CB-CG-CD2	9.08	127.16	120.80
1	A	143	ALA	CA-C-N	9.08	137.17	117.20
1	B	22	TRP	CZ3-CH2-CZ2	9.07	132.49	121.60
1	B	9	ALA	O-C-N	-9.05	108.22	122.70
1	A	78	VAL	CG1-CB-CG2	-9.04	96.43	110.90
1	B	38	LYS	C-N-CD	9.03	147.37	128.40
1	A	145	ALA	O-C-N	9.02	137.13	122.70
1	A	103	PHE	CB-CG-CD2	9.00	127.10	120.80
1	B	159	ARG	CD-NE-CZ	-8.99	111.01	123.60
1	B	16	MET	CA-CB-CG	-8.98	98.03	113.30
1	A	105	PRO	CA-CB-CG	8.96	121.83	104.80
1	B	98	ARG	CG-CD-NE	8.94	130.58	111.80
1	B	74	TRP	CD2-CE3-CZ3	8.87	130.33	118.80
1	A	150	SER	O-C-N	-8.86	108.53	122.70
1	B	50	ILE	C-N-CA	-8.86	103.70	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	TYR	CB-CG-CD2	8.85	126.31	121.00
1	A	72	VAL	CG1-CB-CG2	-8.85	96.74	110.90
1	B	33	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	88	VAL	CG1-CB-CG2	8.83	125.02	110.90
1	B	159	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	79	ASP	CA-C-N	8.76	136.47	117.20
1	B	61	ILE	CG1-CB-CG2	-8.75	92.15	111.40
1	A	69	ASP	OD1-CG-OD2	8.74	139.91	123.30
1	A	85	CYS	C-N-CA	-8.71	104.01	122.30
1	A	33	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	143	ALA	O-C-N	-8.69	108.80	122.70
1	B	157	GLU	CG-CD-OE2	-8.65	100.99	118.30
1	B	101	GLU	CG-CD-OE2	-8.65	101.00	118.30
1	B	18	ASN	CB-CG-ND2	-8.64	95.96	116.70
1	A	79	ASP	CA-C-O	-8.63	101.98	120.10
1	B	100	TYR	CG-CD2-CE2	-8.61	114.41	121.30
1	B	54	LEU	CB-CG-CD1	-8.60	96.38	111.00
1	A	158	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	B	81	ALA	CA-C-N	8.57	136.06	117.20
1	B	31	PHE	CB-CG-CD2	-8.57	114.80	120.80
1	A	23	ASN	CB-CG-OD1	8.56	138.72	121.60
1	B	61	ILE	CA-CB-CG1	8.56	127.27	111.00
1	A	82	ILE	CA-CB-CG2	8.55	128.00	110.90
1	B	96	GLY	CA-C-O	8.55	135.98	120.60
1	A	103	PHE	CZ-CE2-CD2	-8.54	109.85	120.10
1	A	145	ALA	CB-CA-C	8.54	122.90	110.10
1	A	22	TRP	CD2-CE3-CZ3	-8.48	107.78	118.80
1	A	21	PRO	N-CD-CG	8.48	115.92	103.20
1	A	22	TRP	CE3-CZ3-CH2	8.48	130.53	121.20
1	A	110	LEU	CB-CG-CD1	-8.47	96.60	111.00
1	A	92	MET	CG-SD-CE	8.46	113.74	100.20
1	B	100	TYR	CD1-CE1-CZ	8.46	127.42	119.80
1	A	128	TYR	CB-CG-CD2	-8.43	115.94	121.00
1	A	159	ARG	CA-CB-CG	8.42	131.91	113.40
1	A	80	GLU	OE1-CD-OE2	8.39	133.37	123.30
1	B	100	TYR	CD1-CG-CD2	8.35	127.09	117.90
1	B	9	ALA	CA-C-O	8.35	137.64	120.10
1	A	37	ASP	CB-CG-OD2	8.33	125.80	118.30
1	B	88	VAL	CA-CB-CG1	-8.30	98.44	110.90
1	A	10	VAL	CA-CB-CG1	8.29	123.33	110.90
1	B	17	GLU	CA-CB-CG	8.28	131.62	113.40
1	B	84	ALA	N-CA-CB	-8.28	98.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	GLU	OE1-CD-OE2	-8.27	113.37	123.30
1	B	22	TRP	CH2-CZ2-CE2	-8.23	109.17	117.40
1	A	103	PHE	CB-CG-CD1	-8.23	115.04	120.80
1	A	76	LYS	CA-C-N	8.21	135.26	117.20
1	B	133	TRP	NE1-CE2-CZ2	8.21	139.43	130.40
1	B	50	ILE	CA-C-O	-8.21	102.86	120.10
1	B	30	TRP	CB-CG-CD1	8.18	137.63	127.00
1	B	118	GLU	O-C-N	-8.12	109.71	122.70
1	B	103	PHE	CZ-CE2-CD2	8.11	129.84	120.10
1	A	30	TRP	CA-C-O	-8.11	103.07	120.10
1	B	42	MET	O-C-N	8.11	136.98	123.20
1	B	138	SER	N-CA-CB	-8.06	98.40	110.50
1	A	126	PRO	CA-C-N	8.06	134.93	117.20
1	B	33	ARG	CA-C-O	8.06	137.02	120.10
1	A	111	TYR	CD1-CG-CD2	8.06	126.76	117.90
1	A	43	GLY	O-C-N	-8.05	109.83	122.70
1	A	12	ARG	CD-NE-CZ	7.99	134.79	123.60
1	B	65	GLN	CB-CA-C	7.98	126.36	110.40
1	A	90	GLU	CG-CD-OE1	7.98	134.25	118.30
1	B	72	VAL	CA-C-O	-7.95	103.40	120.10
1	A	30	TRP	CA-C-N	7.93	134.65	117.20
1	B	17	GLU	CG-CD-OE2	-7.92	102.46	118.30
1	B	118	GLU	CB-CG-CD	7.92	135.58	114.20
1	A	69	ASP	N-CA-CB	-7.90	96.38	110.60
1	A	44	ARG	NH1-CZ-NH2	-7.88	110.73	119.40
1	B	5	ILE	CA-CB-CG1	-7.87	96.05	111.00
1	B	119	VAL	CG1-CB-CG2	7.85	123.45	110.90
1	B	121	GLY	O-C-N	7.85	135.26	122.70
1	B	72	VAL	CA-C-N	7.84	134.44	117.20
1	A	156	LEU	CB-CG-CD1	7.82	124.30	111.00
1	A	88	VAL	CG1-CB-CG2	-7.78	98.45	110.90
1	B	93	VAL	C-N-CA	7.78	141.15	121.70
1	B	140	PHE	CB-CG-CD2	-7.77	115.36	120.80
1	A	131	ASP	CB-CA-C	-7.76	94.87	110.40
1	B	48	GLU	CA-CB-CG	7.75	130.44	113.40
1	A	12	ARG	CG-CD-NE	7.74	128.05	111.80
1	B	1	MET	CB-CG-SD	7.73	135.58	112.40
1	A	87	ASP	CA-C-N	-7.73	100.20	117.20
1	A	47	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	111	TYR	CD1-CE1-CZ	7.72	126.75	119.80
1	B	159	ARG	NH1-CZ-NH2	7.72	127.89	119.40
1	B	55	PRO	N-CA-C	7.71	132.16	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	OD1-CG-OD2	-7.70	108.67	123.30
1	A	111	TYR	O-C-N	-7.69	110.39	122.70
1	B	122[A]	ASP	N-CA-CB	-7.69	96.77	110.60
1	B	122[B]	ASP	N-CA-CB	-7.69	96.77	110.60
1	B	57	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	55	PRO	O-C-N	-7.68	110.14	123.20
1	B	52	ARG	CA-CB-CG	7.67	130.27	113.40
1	A	69	ASP	CA-C-O	7.66	136.19	120.10
1	A	140	PHE	CG-CD2-CE2	-7.66	112.38	120.80
1	A	21	PRO	CA-N-CD	-7.66	100.78	111.50
1	B	140	PHE	CZ-CE2-CD2	-7.65	110.92	120.10
1	A	144	ASP	O-C-N	-7.64	110.48	122.70
1	A	146	GLN	N-CA-CB	-7.62	96.88	110.60
1	A	152	CYS	CA-C-N	7.62	133.96	117.20
1	B	142	ASP	OD1-CG-OD2	7.62	137.77	123.30
1	B	7	ALA	CB-CA-C	7.59	121.49	110.10
1	B	139	GLU	CG-CD-OE1	7.59	133.49	118.30
1	B	29	ALA	CA-C-N	7.59	133.90	117.20
1	B	55	PRO	C-N-CA	7.59	138.24	122.30
1	A	158	ARG	CG-CD-NE	-7.58	95.88	111.80
1	A	88	VAL	CA-CB-CG2	7.57	122.26	110.90
1	B	122[A]	ASP	OD1-CG-OD2	7.57	137.69	123.30
1	B	122[B]	ASP	OD1-CG-OD2	7.57	137.69	123.30
1	A	47	TRP	CA-C-O	7.57	135.99	120.10
1	B	30	TRP	NE1-CE2-CD2	-7.56	99.74	107.30
1	B	44	ARG	O-C-N	-7.55	110.62	122.70
1	B	30	TRP	NE1-CE2-CZ2	7.55	138.70	130.40
1	B	79	ASP	OD1-CG-OD2	-7.52	109.01	123.30
1	A	158	ARG	CA-C-N	-7.50	100.69	117.20
1	B	60	ILE	CB-CA-C	7.50	126.61	111.60
1	A	142	ASP	O-C-N	7.50	134.70	122.70
1	B	72	VAL	CG1-CB-CG2	7.49	122.88	110.90
1	B	114	HIS	CA-C-N	7.49	133.67	117.20
1	B	65	GLN	CG-CD-OE1	7.45	136.50	121.60
1	A	38	LYS	CA-CB-CG	7.45	129.78	113.40
1	B	105	PRO	CA-N-CD	-7.45	101.07	111.50
1	B	98	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	146	GLN	CG-CD-NE2	7.37	134.40	116.70
1	B	44	ARG	CA-C-O	7.35	135.54	120.10
1	A	55	PRO	C-N-CA	7.34	137.72	122.30
1	A	74	TRP	CA-C-N	7.33	133.33	117.20
1	A	128	TYR	CD1-CE1-CZ	-7.29	113.24	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	47	TRP	CG-CD2-CE3	7.28	140.45	133.90
1	B	104	LEU	CB-CG-CD2	-7.28	98.63	111.00
1	A	159	ARG	CA-C-O	-7.28	104.82	120.10
1	A	30	TRP	CZ3-CH2-CZ2	7.25	130.30	121.60
1	B	53	PRO	O-C-N	-7.23	111.13	122.70
1	B	1	MET	CA-C-O	-7.23	104.93	120.10
1	B	6	ALA	C-N-CA	7.22	139.75	121.70
1	A	61	ILE	CA-CB-CG1	7.20	124.68	111.00
1	B	38	LYS	CD-CE-NZ	-7.19	95.16	111.70
1	A	141	HIS	CG-CD2-NE2	-7.18	95.55	109.20
1	A	128	TYR	CA-C-N	-7.18	101.41	117.20
1	B	68	THR	CA-CB-CG2	7.18	122.45	112.40
1	A	30	TRP	CG-CD2-CE3	-7.16	127.45	133.90
1	A	48	GLU	CB-CA-C	-7.14	96.12	110.40
1	A	116	ASP	OD1-CG-OD2	-7.14	109.73	123.30
1	A	147	ASN	CB-CG-OD1	7.13	135.86	121.60
1	A	114	HIS	N-CA-CB	7.12	123.42	110.60
1	B	70	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	31	PHE	O-C-N	7.11	134.07	122.70
1	B	28	LEU	CB-CG-CD2	7.10	123.08	111.00
1	A	139	GLU	CG-CD-OE2	-7.09	104.11	118.30
1	A	82	ILE	CG1-CB-CG2	-7.06	95.87	111.40
1	A	43	GLY	CA-C-N	7.04	132.70	117.20
1	B	89	PRO	CA-N-CD	7.04	121.55	111.70
1	B	5	ILE	CB-CA-C	7.03	125.67	111.60
1	A	105	PRO	O-C-N	-7.03	111.45	122.70
1	B	68	THR	O-C-N	-7.01	111.49	122.70
1	A	30	TRP	CE3-CZ3-CH2	-7.00	113.50	121.20
1	B	51	GLY	O-C-N	-6.99	111.52	122.70
1	A	10	VAL	O-C-N	-6.96	111.56	122.70
1	B	137	PHE	CD1-CE1-CZ	-6.94	111.78	120.10
1	B	40	VAL	CA-CB-CG1	6.90	121.25	110.90
1	A	121	GLY	C-N-CA	-6.90	104.45	121.70
1	A	36	LEU	CB-CG-CD1	6.89	122.72	111.00
1	A	18	ASN	OD1-CG-ND2	6.87	137.70	121.90
1	A	48	GLU	O-C-N	-6.86	111.73	122.70
1	B	52	ARG	N-CA-CB	-6.85	98.27	110.60
1	B	133	TRP	CD2-CE2-CZ2	-6.84	114.09	122.30
1	B	59	ASN	OD1-CG-ND2	-6.84	106.16	121.90
1	A	22	TRP	CG-CD1-NE1	6.82	116.92	110.10
1	B	13	VAL	CA-CB-CG2	-6.80	100.70	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	PRO	N-CD-CG	6.80	113.40	103.20
1	B	133	TRP	CE3-CZ3-CH2	-6.79	113.72	121.20
1	A	93	VAL	CG1-CB-CG2	6.77	121.73	110.90
1	B	67	GLY	N-CA-C	6.77	130.02	113.10
1	A	151	TYR	C-N-CA	6.77	138.62	121.70
1	B	123	THR	CA-CB-CG2	6.76	121.86	112.40
1	A	100	TYR	O-C-N	6.75	133.50	122.70
1	A	140	PHE	CB-CG-CD1	-6.74	116.08	120.80
1	A	155	ILE	CA-CB-CG1	-6.74	98.19	111.00
1	B	141	HIS	CG-CD2-NE2	-6.74	96.39	109.20
1	B	30	TRP	O-C-N	-6.74	111.92	122.70
1	B	57	ARG	N-CA-CB	-6.72	98.50	110.60
1	A	34	ASN	CA-C-N	6.72	131.98	117.20
1	B	57	ARG	CA-CB-CG	-6.71	98.65	113.40
1	A	120	GLU	CB-CG-CD	6.70	132.28	114.20
1	B	61	ILE	N-CA-CB	6.67	126.14	110.80
1	B	59	ASN	C-N-CA	6.67	138.37	121.70
1	A	125	PHE	CB-CG-CD1	6.66	125.46	120.80
1	A	127	ASP	CB-CA-C	-6.65	97.11	110.40
1	B	118	GLU	CA-C-O	6.63	134.03	120.10
1	A	74	TRP	O-C-N	-6.62	112.10	122.70
1	A	29	ALA	O-C-N	-6.62	112.11	122.70
1	B	53	PRO	N-CA-CB	6.62	111.24	103.30
1	B	80	GLU	N-CA-CB	-6.58	98.75	110.60
1	B	89	PRO	N-CA-CB	-6.58	95.36	102.60
1	A	130	PRO	N-CA-CB	6.58	111.19	103.30
1	B	30	TRP	CB-CG-CD2	-6.56	118.07	126.60
1	A	64[A]	SER	CA-CB-OG	-6.56	93.50	111.20
1	A	64[B]	SER	CA-CB-OG	-6.56	93.50	111.20
1	A	87	ASP	CA-CB-CG	-6.55	98.98	113.40
1	A	155	ILE	N-CA-CB	6.54	125.85	110.80
1	A	150	SER	CB-CA-C	6.54	122.52	110.10
1	A	127	ASP	OD1-CG-OD2	-6.53	110.89	123.30
1	B	1	MET	C-N-CA	-6.52	105.39	121.70
1	A	105	PRO	CA-C-O	6.52	135.84	120.20
1	B	6	ALA	CA-C-N	6.52	131.54	117.20
1	A	78	VAL	CA-C-O	6.52	133.79	120.10
1	A	129	GLU	CB-CA-C	6.51	123.42	110.40
1	B	23	ASN	CA-C-N	-6.51	102.88	117.20
1	A	144	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	54	LEU	O-C-N	6.49	133.43	121.10
1	B	116	ASP	OD1-CG-OD2	6.49	135.62	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PHE	CD1-CG-CD2	6.48	126.72	118.30
1	A	30	TRP	CG-CD1-NE1	-6.47	103.63	110.10
1	A	120	GLU	CA-C-N	6.45	129.10	116.20
1	B	58	LYS	CD-CE-NZ	6.44	126.50	111.70
1	A	87	ASP	CA-C-O	6.43	133.60	120.10
1	A	52	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	A	111	TYR	C-N-CA	6.42	137.74	121.70
1	A	151	TYR	CB-CG-CD2	6.41	124.85	121.00
1	A	107	ALA	CA-C-O	6.40	133.55	120.10
1	B	59	ASN	CA-C-O	-6.40	106.66	120.10
1	B	106	LYS	CB-CG-CD	6.40	128.24	111.60
1	A	65	GLN	O-C-N	-6.39	108.95	121.10
1	A	132	ASP	CB-CG-OD1	6.39	124.06	118.30
1	B	46	THR	CA-CB-CG2	6.39	121.35	112.40
1	B	157	GLU	OE1-CD-OE2	6.37	130.94	123.30
1	B	111	TYR	CZ-CE2-CD2	-6.36	114.07	119.80
1	A	153	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	B	137	PHE	O-C-N	6.34	132.85	122.70
1	A	48	GLU	CA-CB-CG	6.33	127.33	113.40
1	A	133	TRP	NE1-CE2-CZ2	-6.33	123.44	130.40
1	A	158	ARG	CB-CG-CD	-6.33	95.16	111.60
1	B	78	VAL	CA-CB-CG2	-6.32	101.42	110.90
1	B	120	GLU	OE1-CD-OE2	6.32	130.89	123.30
1	B	16	MET	O-C-N	-6.32	112.59	122.70
1	B	149	HIS	CA-CB-CG	6.31	124.33	113.60
1	B	47	TRP	N-CA-CB	-6.31	99.25	110.60
1	A	158	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
1	B	54	LEU	C-N-CD	6.30	141.62	128.40
1	B	134	GLU	CG-CD-OE2	-6.29	105.73	118.30
1	A	80	GLU	CB-CA-C	-6.29	97.83	110.40
1	B	24	LEU	CB-CG-CD2	-6.28	100.33	111.00
1	B	7	ALA	CA-C-N	6.28	131.01	117.20
1	B	137	PHE	CA-C-N	-6.26	103.42	117.20
1	A	47	TRP	CD2-CE3-CZ3	6.24	126.91	118.80
1	B	86	GLY	CA-C-N	-6.22	103.51	117.20
1	B	71	ARG	NH1-CZ-NH2	6.22	126.24	119.40
1	A	25	PRO	O-C-N	-6.21	112.76	122.70
1	A	109	LYS	C-N-CA	6.20	137.20	121.70
1	A	11	ASP	OD1-CG-OD2	-6.19	111.54	123.30
1	B	101	GLU	CA-C-O	6.18	133.09	120.10
1	A	37	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	B	44	ARG	N-CA-C	6.17	127.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LEU	CA-C-O	6.17	133.06	120.10
1	B	59	ASN	CB-CG-OD1	6.16	133.93	121.60
1	A	126	PRO	O-C-N	-6.16	112.84	122.70
1	A	80	GLU	N-CA-CB	-6.16	99.51	110.60
1	B	125	PHE	CB-CG-CD1	6.16	125.11	120.80
1	B	16	MET	CA-C-O	6.16	133.03	120.10
1	A	150	SER	C-N-CA	6.15	137.08	121.70
1	A	132	ASP	N-CA-CB	-6.15	99.53	110.60
1	B	55	PRO	CA-C-O	-6.14	105.47	120.20
1	A	125	PHE	C-N-CD	6.12	141.26	128.40
1	A	32	LYS	O-C-N	6.12	132.49	122.70
1	B	79	ASP	O-C-N	-6.12	112.91	122.70
1	B	141	HIS	ND1-CG-CD2	6.11	117.35	108.80
1	A	47	TRP	CA-C-N	-6.10	103.79	117.20
1	B	74	TRP	CD1-CG-CD2	-6.10	101.42	106.30
1	A	93	VAL	CA-CB-CG2	-6.07	101.79	110.90
1	A	17	GLU	O-C-N	6.07	132.41	122.70
1	B	154	LYS	CB-CG-CD	-6.07	95.83	111.60
1	B	25	PRO	O-C-N	-6.06	113.00	122.70
1	A	152	CYS	O-C-N	-6.05	113.02	122.70
1	A	103	PHE	O-C-N	-6.04	113.03	122.70
1	B	103	PHE	CG-CD2-CE2	-6.02	114.17	120.80
1	B	14	ILE	O-C-N	-6.02	112.97	123.20
1	A	135	SER	CB-CA-C	-6.01	98.69	110.10
1	B	153	PHE	CZ-CE2-CD2	-6.01	112.89	120.10
1	A	141	HIS	ND1-CG-CD2	6.00	117.21	108.80
1	A	37	ASP	N-CA-CB	5.99	121.39	110.60
1	A	46	THR	N-CA-CB	5.99	121.69	110.30
1	A	125	PHE	CA-C-O	-5.98	107.55	120.10
1	B	45[A]	HIS	CA-CB-CG	-5.96	103.46	113.60
1	B	45[B]	HIS	CA-CB-CG	-5.96	103.46	113.60
1	A	69	ASP	N-CA-C	5.95	127.07	111.00
1	A	141	HIS	CE1-NE2-CD2	5.95	121.47	106.60
1	A	157	GLU	CB-CG-CD	5.95	130.26	114.20
1	A	141	HIS	O-C-N	-5.94	113.20	122.70
1	B	74	TRP	CH2-CZ2-CE2	-5.92	111.48	117.40
1	A	87	ASP	OD1-CG-OD2	5.92	134.55	123.30
1	A	152	CYS	C-N-CA	5.92	136.50	121.70
1	B	157	GLU	CA-CB-CG	5.92	126.41	113.40
1	A	27	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	26	ALA	CA-C-O	5.88	132.45	120.10
1	B	141	HIS	CA-C-O	5.88	132.44	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	GLU	CA-C-O	5.88	132.44	120.10
1	B	36	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	B	31	PHE	CA-C-O	-5.86	107.80	120.10
1	B	53	PRO	CA-CB-CG	-5.86	92.87	104.00
1	B	154	LYS	CD-CE-NZ	-5.85	98.25	111.70
1	B	53	PRO	CA-C-O	5.84	134.22	120.20
1	B	31	PHE	CB-CG-CD1	5.84	124.89	120.80
1	B	96	GLY	CA-C-N	-5.83	104.54	116.20
1	A	79	ASP	N-CA-CB	-5.83	100.11	110.60
1	A	125	PHE	O-C-N	5.83	132.17	121.10
1	A	40	VAL	O-C-N	5.82	132.01	122.70
1	A	133	TRP	CH2-CZ2-CE2	-5.82	111.58	117.40
1	A	44	ARG	CA-C-N	5.81	129.98	117.20
1	A	34	ASN	O-C-N	-5.80	113.43	122.70
1	A	100	TYR	CD1-CG-CD2	5.79	124.27	117.90
1	B	119	VAL	CA-CB-CG2	5.79	119.59	110.90
1	A	74	TRP	CD1-NE1-CE2	5.79	114.21	109.00
1	B	2	ILE	CA-CB-CG2	5.79	122.47	110.90
1	A	3	SER	N-CA-CB	5.78	119.17	110.50
1	B	62	LEU	N-CA-CB	5.78	121.97	110.40
1	A	133	TRP	CD1-NE1-CE2	-5.78	103.80	109.00
1	B	109	LYS	CD-CE-NZ	5.78	124.98	111.70
1	B	139	GLU	OE1-CD-OE2	-5.77	116.37	123.30
1	A	44	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	74	TRP	C-N-CA	5.75	136.08	121.70
1	B	83	ALA	N-CA-CB	-5.75	102.05	110.10
1	B	65	GLN	OE1-CD-NE2	-5.75	108.67	121.90
1	B	34	ASN	CB-CG-OD1	5.74	133.07	121.60
1	A	158	ARG	N-CA-CB	5.73	120.91	110.60
1	B	20	MET	N-CA-CB	5.72	120.91	110.60
1	B	115	ILE	O-C-N	5.71	131.84	122.70
1	A	47	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	B	135	SER	CA-C-N	5.70	129.74	117.20
1	B	112	LEU	O-C-N	5.69	131.81	122.70
1	A	53	PRO	N-CA-CB	5.69	110.12	103.30
1	A	54	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	B	81	ALA	CB-CA-C	5.68	118.62	110.10
1	B	145	ALA	CB-CA-C	-5.68	101.58	110.10
1	A	140	PHE	O-C-N	5.68	131.78	122.70
1	A	156	LEU	O-C-N	-5.67	113.62	122.70
1	B	24	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	B	151	TYR	CA-C-O	-5.67	108.20	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45[A]	HIS	O-C-N	-5.66	113.64	122.70
1	B	45[B]	HIS	O-C-N	-5.66	113.64	122.70
1	A	104	LEU	CB-CG-CD1	5.66	120.62	111.00
1	B	45[A]	HIS	CG-CD2-NE2	-5.66	98.45	109.20
1	B	45[B]	HIS	CG-CD2-NE2	-5.66	98.45	109.20
1	A	158	ARG	CB-CA-C	-5.65	99.11	110.40
1	A	81	ALA	CA-C-O	-5.64	108.25	120.10
1	A	78	VAL	CA-C-N	-5.64	104.79	117.20
1	B	113	THR	CA-CB-CG2	5.63	120.29	112.40
1	B	120	GLU	C-N-CA	-5.63	110.47	122.30
1	A	103	PHE	CE1-CZ-CE2	5.63	130.13	120.00
1	A	74	TRP	CB-CG-CD1	-5.63	119.69	127.00
1	A	29	ALA	N-CA-CB	-5.62	102.22	110.10
1	B	133	TRP	CH2-CZ2-CE2	5.62	123.02	117.40
1	A	24	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	B	17	GLU	CB-CG-CD	5.60	129.32	114.20
1	B	100	TYR	CE1-CZ-CE2	5.60	128.76	119.80
1	B	97	GLY	N-CA-C	5.59	127.09	113.10
1	B	8	LEU	CB-CG-CD2	5.59	120.51	111.00
1	A	18	ASN	CB-CG-ND2	-5.59	103.28	116.70
1	A	112	LEU	CB-CG-CD2	5.57	120.47	111.00
1	B	23	ASN	N-CA-CB	-5.57	100.58	110.60
1	B	140	PHE	CA-C-O	5.56	131.78	120.10
1	A	32	LYS	N-CA-CB	-5.55	100.61	110.60
1	A	140	PHE	CD1-CG-CD2	5.54	125.50	118.30
1	B	44	ARG	CD-NE-CZ	-5.53	115.86	123.60
1	A	151	TYR	CG-CD1-CE1	5.53	125.72	121.30
1	A	154	LYS	CB-CG-CD	5.53	125.97	111.60
1	A	11	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	30	TRP	CE2-CD2-CG	5.52	111.72	107.30
1	A	100	TYR	CD1-CE1-CZ	5.49	124.74	119.80
1	B	134	GLU	CG-CD-OE1	5.48	129.26	118.30
1	B	98	ARG	CB-CA-C	-5.48	99.44	110.40
1	B	45[A]	HIS	CE1-NE2-CD2	5.48	120.30	106.60
1	B	45[B]	HIS	CE1-NE2-CD2	5.48	120.30	106.60
1	A	31	PHE	CD1-CE1-CZ	-5.47	113.53	120.10
1	A	82	ILE	N-CA-CB	5.47	123.39	110.80
1	A	100	TYR	CA-C-N	-5.46	105.18	117.20
1	A	6	ALA	CA-C-O	5.46	131.56	120.10
1	A	76	LYS	CA-C-O	-5.45	108.65	120.10
1	B	18	ASN	N-CA-CB	-5.45	100.78	110.60
1	A	144	ASP	CA-C-N	5.45	129.19	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LYS	CA-CB-CG	-5.45	101.42	113.40
1	B	97	GLY	CA-C-O	5.44	130.39	120.60
1	B	133	TRP	CD1-NE1-CE2	5.43	113.89	109.00
1	B	144	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	62	LEU	CD1-CG-CD2	-5.43	94.21	110.50
1	A	23	ASN	CB-CG-ND2	-5.42	103.70	116.70
1	B	86	GLY	O-C-N	5.41	131.35	122.70
1	B	126	PRO	CA-C-O	5.41	133.18	120.20
1	B	22	TRP	NE1-CE2-CZ2	-5.40	124.46	130.40
1	B	89	PRO	N-CA-C	5.39	126.12	112.10
1	B	42	MET	C-N-CA	-5.39	110.98	122.30
1	B	48	GLU	CB-CG-CD	5.38	128.73	114.20
1	A	122	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	142	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	12	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	128	TYR	O-C-N	5.35	131.27	122.70
1	B	158	ARG	C-N-CA	-5.35	108.33	121.70
1	A	45	HIS	CE1-NE2-CD2	5.35	119.97	106.60
1	A	150	SER	CA-C-O	5.35	131.33	120.10
1	B	105	PRO	CB-CG-CD	-5.34	85.66	106.50
1	B	130	PRO	O-C-N	5.34	131.25	122.70
1	A	74	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	A	89	PRO	CB-CA-C	-5.33	98.66	112.00
1	B	127	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	103	PHE	CG-CD2-CE2	5.33	126.67	120.80
1	B	8	LEU	O-C-N	-5.33	114.17	122.70
1	A	68	THR	O-C-N	-5.33	114.17	122.70
1	B	158	ARG	CG-CD-NE	-5.32	100.62	111.80
1	A	62	LEU	O-C-N	-5.32	114.20	122.70
1	B	61	ILE	CA-CB-CG2	5.31	121.52	110.90
1	A	71	ARG	N-CA-CB	-5.31	101.04	110.60
1	B	43	GLY	CA-C-O	5.31	130.16	120.60
1	B	74	TRP	CB-CG-CD2	5.30	133.49	126.60
1	B	31	PHE	CG-CD2-CE2	-5.30	114.97	120.80
1	B	156	LEU	CA-C-N	-5.30	105.54	117.20
1	B	2	ILE	CA-CB-CG1	-5.29	100.94	111.00
1	A	14	ILE	C-N-CA	-5.29	111.19	122.30
1	A	47	TRP	C-N-CA	-5.29	108.48	121.70
1	B	130	PRO	N-CA-CB	5.28	109.64	103.30
1	A	14	ILE	O-C-N	5.27	132.16	123.20
1	A	154	LYS	CG-CD-CE	5.26	127.70	111.90
1	B	40	VAL	O-C-N	5.26	131.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	LYS	CD-CE-NZ	-5.26	99.61	111.70
1	A	12	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	A	17	GLU	CA-CB-CG	5.25	124.96	113.40
1	B	15	GLY	O-C-N	5.25	131.10	122.70
1	B	59	ASN	O-C-N	-5.25	114.30	122.70
1	A	45	HIS	ND1-CE1-NE2	-5.24	98.37	109.90
1	B	135	SER	C-N-CA	5.24	134.80	121.70
1	B	102	GLN	N-CA-CB	-5.23	101.19	110.60
1	A	153	PHE	CA-C-O	-5.22	109.13	120.10
1	B	153	PHE	CA-C-O	-5.22	109.14	120.10
1	B	141	HIS	O-C-N	-5.21	114.36	122.70
1	B	57	ARG	CB-CA-C	-5.19	100.02	110.40
1	A	44	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	74	TRP	NE1-CE2-CD2	-5.18	102.12	107.30
1	A	84	ALA	N-CA-CB	5.18	117.36	110.10
1	A	98	ARG	CA-CB-CG	-5.18	102.00	113.40
1	A	114	HIS	CG-ND1-CE1	5.18	115.45	108.20
1	B	82	ILE	CB-CG1-CD1	5.17	128.39	113.90
1	A	134	GLU	O-C-N	-5.17	114.43	122.70
1	B	28	LEU	CA-C-O	-5.17	109.24	120.10
1	A	4	LEU	N-CA-CB	5.16	120.73	110.40
1	A	103	PHE	CA-C-N	5.16	128.56	117.20
1	A	88	VAL	CA-C-N	-5.16	102.65	117.10
1	B	17	GLU	N-CA-CB	-5.16	101.31	110.60
1	A	21	PRO	N-CA-CB	5.16	109.49	103.30
1	A	58	LYS	CD-CE-NZ	-5.15	99.86	111.70
1	A	142	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	9	ALA	N-CA-C	-5.15	97.10	111.00
1	B	33	ARG	CA-C-N	-5.15	105.88	117.20
1	B	148	SER	N-CA-CB	-5.14	102.79	110.50
1	A	82	ILE	CA-C-O	5.14	130.89	120.10
1	A	1	MET	N-CA-C	-5.13	97.15	111.00
1	B	65	GLN	CA-C-O	5.13	130.87	120.10
1	A	61	ILE	CB-CG1-CD1	5.12	128.25	113.90
1	A	36	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	B	104	LEU	N-CA-CB	5.12	120.64	110.40
1	A	52	ARG	C-N-CD	5.10	139.11	128.40
1	A	74	TRP	CH2-CZ2-CE2	-5.10	112.30	117.40
1	B	103	PHE	O-C-N	5.10	130.86	122.70
1	B	146	GLN	CA-CB-CG	-5.10	102.17	113.40
1	B	76	LYS	N-CA-CB	-5.10	101.42	110.60
1	B	22	TRP	CD1-NE1-CE2	-5.10	104.41	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	TRP	CA-CB-CG	5.10	123.39	113.70
1	B	26	ALA	O-C-N	-5.10	114.55	122.70
1	B	38	LYS	CA-C-N	-5.09	102.84	117.10
1	B	145	ALA	O-C-N	5.09	130.85	122.70
1	A	77	SER	C-N-CA	5.09	134.42	121.70
1	A	103	PHE	CG-CD1-CE1	-5.09	115.20	120.80
1	A	124	HIS	C-N-CA	5.09	134.43	121.70
1	B	14	ILE	N-CA-CB	5.08	122.49	110.80
1	A	44	ARG	CA-C-O	-5.08	109.43	120.10
1	B	23	ASN	CA-CB-CG	-5.08	102.23	113.40
1	A	54	LEU	O-C-N	5.08	130.75	121.10
1	B	7	ALA	CA-C-O	-5.08	109.44	120.10
1	B	132	ASP	O-C-N	5.07	130.81	122.70
1	B	140	PHE	CA-C-N	-5.06	106.07	117.20
1	A	109	LYS	CG-CD-CE	5.05	127.05	111.90
1	A	46	THR	CA-CB-OG1	-5.04	98.41	109.00
1	A	133	TRP	C-N-CA	5.03	134.28	121.70
1	B	18	ASN	CA-C-O	5.00	130.61	120.10
1	B	44	ARG	N-CA-CB	-5.00	101.59	110.60
1	A	144	ASP	C-N-CA	5.00	134.20	121.70

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ALA	Mainchain
1	A	33	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	65	GLN	Mainchain,Peptide
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

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Mol	Chain	Res	Type	Group
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	1175	24	0
1	B	1286	0	1217	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	33	0	19	2	0
4	B	33	0	20	0	0
5	A	239	0	0	11	0
5	B	189	0	0	9	0
All	All	3035	0	2431	57	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 11.

All (57) 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:CB	1:B:57:ARG:CA	1.74	1.61
1:A:58:LYS:CE	1:A:58:LYS:CD	1.75	1.57
1:A:109:LYS:NZ	1:A:109:LYS:CE	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	1.32
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:N	1:B:159:ARG:CB	2.40	0.84
1:B:57:ARG:N	1:B:57:ARG:CB	2.42	0.81
1:B:158:ARG:C	1:B:159:ARG:CA	2.49	0.80
1:A:46:THR:OG1	5:A:376:HOH:O	2.05	0.75
1:B:57:ARG:CB	1:B:57:ARG:C	2.56	0.73
1:A:58:LYS:CD	1:A:58:LYS:NZ	2.54	0.71
1:B:108:GLN:HG2	5:B:181:HOH:O	1.93	0.68
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:B:159:ARG:C	1:B:159:ARG:N	2.54	0.58
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: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
1:A:95:GLY:C	5:A:376:HOH:O	2.46	0.53
4: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:HG3	1:B:57:ARG:CA	2.42	0.48
1:A:44:ARG:HG3	1:A:44:ARG:O	2.15	0.47
1:A:27:ASP:OD2	4:A:161:MTX:N1	2.48	0.46
1:B:64[A]:SER:CB	1:B:65:GLN:HE21	2.28	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:CG2	5:A:376:HOH:O	2.69	0.41
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:B:44:ARG:HH12	1:B:68:THR:CG2	2.34	0.40
1:A:54:LEU:HA	1:A:55:PRO:HD3	1.96	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%)	15	2
1	B	160/159 (101%)	156 (98%)	4 (2%)	0	100	100
All	All	318/318 (100%)	302 (95%)	14 (4%)	2 (1%)	30	12

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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%)	117 (90%)	13 (10%)	9	2
1	B	137/136 (101%)	129 (94%)	8 (6%)	25	8
All	All	267/272 (98%)	246 (92%)	21 (8%)	16	3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
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	61	ILE
1	B	68	THR
1	B	111	TYR
1	B	118	GLU
1	B	158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	MTX	A	161	-	27,35,35	2.99	12 (44%)	30,49,49	3.16	14 (46%)
4	MTX	B	162	-	27,35,35	2.73	12 (44%)	30,49,49	3.49	12 (40%)

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
4	MTX	A	161	-	-	0/19/25/25	0/3/3/3
4	MTX	B	162	-	-	0/19/25/25	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	162	MTX	C7-C6	-6.16	1.28	1.39
4	A	161	MTX	C4-NA4	-3.57	1.23	1.34
4	A	161	MTX	C16-C11	-3.46	1.33	1.39
4	B	162	MTX	CA-N	-3.13	1.42	1.46
4	B	162	MTX	CB-CA	-2.59	1.49	1.53
4	B	162	MTX	C16-C15	-2.46	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	161	MTX	C13-C14	-2.45	1.34	1.39
4	A	161	MTX	C2-N3	-2.13	1.31	1.35
4	B	162	MTX	C16-C11	2.08	1.42	1.39
4	B	162	MTX	C7-N8	2.10	1.35	1.31
4	B	162	MTX	C8A-N8	2.21	1.40	1.37
4	B	162	MTX	CB-CG	2.62	1.65	1.52
4	A	161	MTX	C15-C14	3.22	1.45	1.39
4	A	161	MTX	C8A-N8	3.61	1.43	1.37
4	B	162	MTX	C2-NA2	3.75	1.41	1.34
4	B	162	MTX	C8A-N1	4.22	1.44	1.36
4	A	161	MTX	C9-N10	4.29	1.53	1.47
4	A	161	MTX	C14-N10	4.76	1.54	1.39
4	A	161	MTX	C7-C6	4.90	1.47	1.39
4	B	162	MTX	CM-N10	5.00	1.54	1.46
4	A	161	MTX	CM-N10	5.17	1.54	1.46
4	A	161	MTX	O-C	5.33	1.34	1.23
4	B	162	MTX	C9-N10	6.84	1.57	1.47
4	A	161	MTX	CA-N	6.97	1.56	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	162	MTX	C7-N8-C8A	-10.36	104.72	116.93
4	A	161	MTX	N8-C8A-N1	-7.77	105.02	116.14
4	B	162	MTX	C15-C16-C11	-5.92	113.90	120.76
4	A	161	MTX	C11-C-N	-5.83	106.55	116.93
4	A	161	MTX	CG-CB-CA	-5.26	102.30	112.99
4	B	162	MTX	CM-N10-C9	-4.58	101.83	114.23
4	B	162	MTX	C13-C14-N10	-4.35	115.08	121.68
4	A	161	MTX	C12-C13-C14	-3.48	115.86	120.36
4	A	161	MTX	C15-C16-C11	-3.33	116.90	120.76
4	B	162	MTX	C13-C12-C11	-3.31	116.92	120.76
4	B	162	MTX	CG-CB-CA	-3.01	106.86	112.99
4	B	162	MTX	C6-N5-C4A	-2.59	112.16	117.62
4	B	162	MTX	N8-C8A-N1	-2.46	112.62	116.14
4	A	161	MTX	NA2-C2-N1	-2.25	113.49	117.80
4	B	162	MTX	C12-C11-C	-2.14	113.80	120.60
4	A	161	MTX	C16-C15-C14	2.29	123.33	120.36
4	A	161	MTX	C9-N10-C14	3.36	126.52	119.36
4	A	161	MTX	NA4-C4-N3	3.41	127.83	116.45
4	A	161	MTX	C2-N3-C4	3.49	127.73	116.70
4	A	161	MTX	C13-C12-C11	3.81	125.18	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	162	MTX	CB-CG-CD	4.10	129.72	113.02
4	A	161	MTX	O-C-N	4.49	130.56	122.44
4	A	161	MTX	C4A-C8A-N1	4.90	130.03	122.11
4	B	162	MTX	C16-C11-C12	4.95	125.95	118.60
4	A	161	MTX	CB-CG-CD	5.52	135.52	113.02
4	B	162	MTX	CM-N10-C14	8.73	134.54	119.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.