



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:57 PM UTC

PDB ID : 3DFR / pdb_00003dfr
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

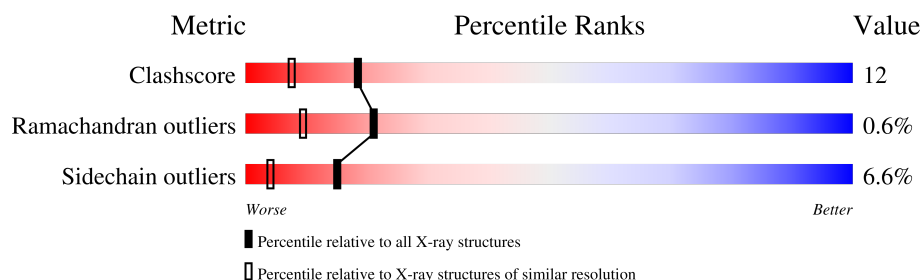
1 Overall quality at a glance

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	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTX	A	164	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1639 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.

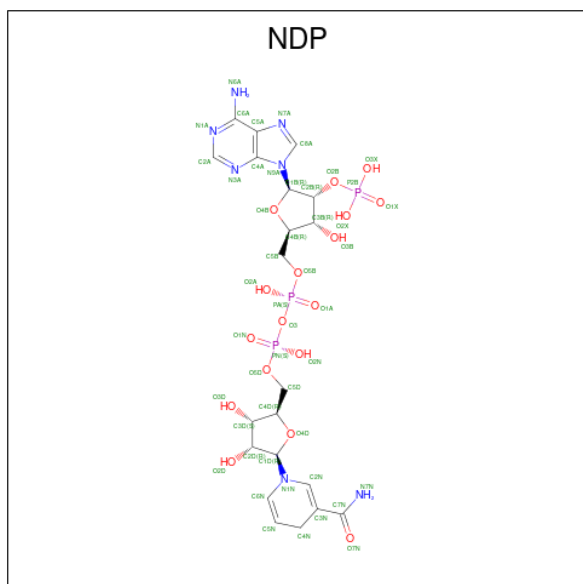
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1294	826	226	240	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

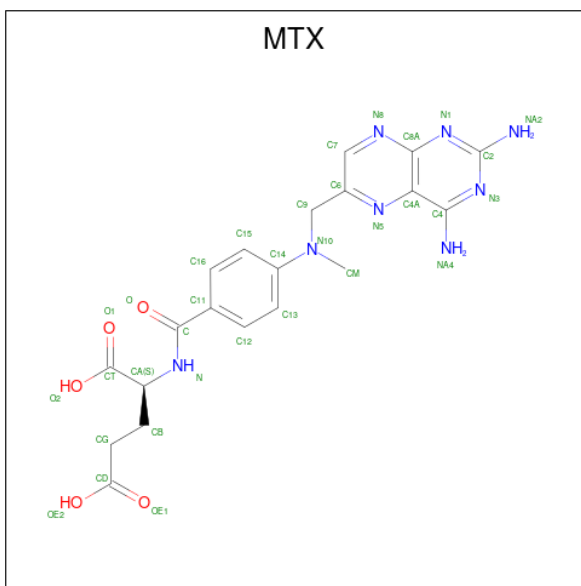
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASN	ASP	conflict	UNP P00381
A	10	ASN	ASP	conflict	UNP P00381
A	90	LEU	PRO	conflict	UNP P00381

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$).



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

- Molecule 4 is water.

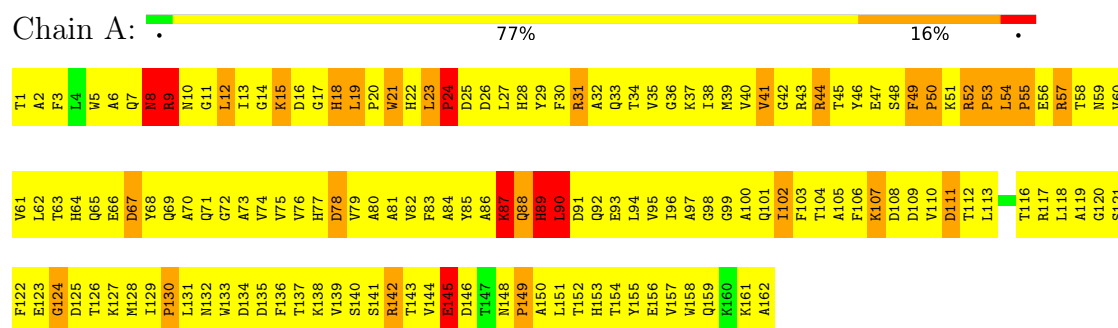
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	264	Total O 264 264	0	0

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



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	71.86Å 71.86Å 93.38Å 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}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1639	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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, NDP

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	4.62	265/1328 (20.0%)	5.39	510/1809 (28.2%)

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	1	8

All (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	HIS	C-O	26.70	1.57	1.24
1	A	89	HIS	C-N	-26.27	0.96	1.33
1	A	19	LEU	C-N	23.38	1.55	1.33
1	A	50	PRO	N-CD	22.18	1.78	1.47
1	A	24	PRO	N-CD	21.89	1.78	1.47
1	A	18	HIS	CD2-NE2	21.79	1.61	1.37
1	A	142	ARG	NE-CZ	19.89	1.54	1.33
1	A	67	ASP	CA-CB	19.71	1.87	1.53
1	A	54	LEU	C-N	19.50	1.57	1.33
1	A	130	PRO	N-CD	18.13	1.73	1.47
1	A	129	ILE	C-N	17.98	1.54	1.33
1	A	149	PRO	N-CD	16.29	1.70	1.47
1	A	52	ARG	C-N	16.06	1.64	1.34
1	A	117	ARG	NE-CZ	-15.72	1.15	1.33
1	A	148	ASN	C-N	15.34	1.51	1.34
1	A	55	PRO	N-CD	15.31	1.69	1.47
1	A	53	PRO	N-CD	15.00	1.68	1.47
1	A	28	HIS	CG-CD2	14.66	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LEU	N-CA	14.39	1.64	1.46
1	A	105	ALA	C-O	14.16	1.42	1.24
1	A	23	LEU	C-O	-13.43	1.09	1.24
1	A	135	ASP	CA-C	13.17	1.71	1.52
1	A	67	ASP	CG-OD1	13.10	1.50	1.25
1	A	18	HIS	CG-ND1	13.06	1.52	1.38
1	A	20	PRO	N-CD	13.05	1.66	1.47
1	A	31	ARG	NE-CZ	12.92	1.47	1.33
1	A	145	GLU	CD-OE2	12.90	1.49	1.25
1	A	18	HIS	ND1-CE1	12.85	1.45	1.32
1	A	49	PHE	C-N	12.84	1.50	1.34
1	A	78	ASP	C-O	12.75	1.38	1.23
1	A	90	LEU	CG-CD2	12.68	1.94	1.52
1	A	23	LEU	C-N	12.45	1.50	1.34
1	A	10	ASN	CG-OD1	12.24	1.46	1.23
1	A	90	LEU	CB-CG	-12.00	1.29	1.53
1	A	67	ASP	CG-OD2	11.81	1.47	1.25
1	A	95	VAL	CA-C	11.74	1.68	1.52
1	A	77	HIS	CE1-NE2	11.71	1.44	1.32
1	A	148	ASN	CA-C	11.67	1.66	1.52
1	A	67	ASP	C-N	11.26	1.48	1.33
1	A	146	ASP	CA-C	11.25	1.66	1.52
1	A	90	LEU	CG-CD1	10.97	1.88	1.52
1	A	117	ARG	CZ-NH1	10.97	1.48	1.32
1	A	14	GLY	CA-C	10.84	1.63	1.51
1	A	49	PHE	CA-C	10.75	1.64	1.53
1	A	19	LEU	C-O	-10.71	1.10	1.23
1	A	142	ARG	CA-C	10.61	1.65	1.52
1	A	22	HIS	CG-CD2	10.56	1.47	1.35
1	A	64	HIS	CG-ND1	-10.55	1.26	1.38
1	A	94	LEU	CA-C	10.43	1.65	1.52
1	A	16	ASP	CA-CB	10.37	1.69	1.53
1	A	148	ASN	C-O	-10.37	1.11	1.24
1	A	20	PRO	N-CA	10.36	1.59	1.47
1	A	132	ASN	N-CA	10.31	1.59	1.46
1	A	50	PRO	CA-CB	10.27	1.69	1.53
1	A	44	ARG	CD-NE	-10.11	1.32	1.46
1	A	58	THR	CA-CB	10.08	1.66	1.53
1	A	134	ASP	CG-OD1	9.86	1.44	1.25
1	A	91	ASP	CA-CB	9.71	1.71	1.53
1	A	23	LEU	CA-C	9.70	1.64	1.52
1	A	55	PRO	N-CA	9.66	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ASP	CA-CB	9.59	1.69	1.53
1	A	152	THR	CA-C	9.51	1.65	1.52
1	A	78	ASP	CG-OD2	9.48	1.43	1.25
1	A	8	ASN	N-CA	9.40	1.57	1.45
1	A	134	ASP	CG-OD2	9.38	1.43	1.25
1	A	91	ASP	C-N	9.34	1.45	1.33
1	A	11	GLY	C-N	9.26	1.45	1.33
1	A	123	GLU	CA-CB	9.12	1.67	1.53
1	A	25	ASP	C-O	-9.10	1.13	1.24
1	A	44	ARG	CZ-NH1	9.02	1.45	1.32
1	A	137	THR	C-O	8.95	1.34	1.24
1	A	77	HIS	CA-CB	8.94	1.67	1.53
1	A	83	PHE	C-N	-8.93	1.22	1.33
1	A	50	PRO	N-CA	8.91	1.59	1.47
1	A	86	ALA	CA-C	8.85	1.64	1.52
1	A	88	GLN	C-N	8.82	1.46	1.33
1	A	70	ALA	C-O	8.75	1.33	1.23
1	A	108	ASP	CB-CG	8.73	1.73	1.52
1	A	139	VAL	CA-CB	8.68	1.66	1.54
1	A	10	ASN	CB-CG	8.68	1.73	1.52
1	A	142	ARG	CZ-NH1	8.54	1.44	1.32
1	A	145	GLU	CD-OE1	8.54	1.41	1.25
1	A	30	PHE	C-O	-8.51	1.14	1.24
1	A	51	LYS	CA-CB	8.51	1.69	1.53
1	A	75	VAL	C-N	8.50	1.44	1.33
1	A	54	LEU	C-O	-8.50	1.12	1.23
1	A	6	ALA	N-CA	8.49	1.56	1.46
1	A	81	ALA	CA-C	-8.47	1.41	1.52
1	A	79	VAL	CA-CB	8.41	1.66	1.54
1	A	145	GLU	CB-CG	8.38	1.77	1.52
1	A	144	VAL	CA-C	8.35	1.63	1.52
1	A	129	ILE	C-O	-8.34	1.14	1.24
1	A	51	LYS	N-CA	8.28	1.56	1.46
1	A	60	VAL	C-N	-8.21	1.23	1.33
1	A	63	THR	C-O	8.18	1.33	1.23
1	A	13	ILE	C-N	8.17	1.45	1.33
1	A	64	HIS	ND1-CE1	8.10	1.40	1.32
1	A	39	MET	N-CA	-8.08	1.36	1.46
1	A	161	LYS	C-N	8.07	1.44	1.33
1	A	140	SER	CA-CB	8.04	1.70	1.54
1	A	65	GLN	CD-NE2	8.03	1.50	1.33
1	A	17	GLY	N-CA	8.01	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	LEU	C-O	7.95	1.33	1.23
1	A	162	ALA	C-O	7.92	1.39	1.23
1	A	92	GLN	CA-C	7.92	1.62	1.52
1	A	91	ASP	C-O	7.86	1.34	1.24
1	A	24	PRO	CA-CB	7.84	1.65	1.53
1	A	49	PHE	CG-CD2	7.83	1.55	1.38
1	A	82	VAL	N-CA	-7.82	1.37	1.46
1	A	111	ASP	N-CA	7.80	1.55	1.45
1	A	91	ASP	CA-C	7.78	1.63	1.52
1	A	70	ALA	CA-CB	7.76	1.62	1.52
1	A	123	GLU	CA-C	-7.75	1.43	1.52
1	A	132	ASN	C-O	7.72	1.34	1.23
1	A	149	PRO	C-O	7.71	1.34	1.24
1	A	141	SER	C-O	7.66	1.32	1.23
1	A	142	ARG	N-CA	7.63	1.55	1.46
1	A	109	ASP	CB-CG	7.57	1.71	1.52
1	A	25	ASP	N-CA	-7.56	1.37	1.46
1	A	48	SER	C-N	7.55	1.44	1.33
1	A	98	GLY	C-O	-7.54	1.16	1.24
1	A	108	ASP	CG-OD2	7.46	1.39	1.25
1	A	57	ARG	CA-CB	7.36	1.65	1.53
1	A	44	ARG	CA-C	-7.28	1.43	1.52
1	A	125	ASP	CG-OD1	7.28	1.39	1.25
1	A	76	VAL	C-N	7.22	1.44	1.33
1	A	32	ALA	C-O	-7.19	1.15	1.24
1	A	22	HIS	C-O	-7.17	1.14	1.23
1	A	118	LEU	CB-CG	7.17	1.67	1.53
1	A	162	ALA	CA-C	7.16	1.68	1.52
1	A	30	PHE	CA-CB	7.10	1.64	1.53
1	A	22	HIS	CE1-NE2	7.10	1.39	1.32
1	A	91	ASP	CG-OD2	7.08	1.38	1.25
1	A	69	GLN	C-O	-7.07	1.15	1.24
1	A	32	ALA	C-N	7.05	1.44	1.33
1	A	121	SER	CB-OG	-7.04	1.28	1.42
1	A	45	THR	CA-C	6.99	1.61	1.52
1	A	162	ALA	C-OXT	6.93	1.37	1.23
1	A	111	ASP	CG-OD1	6.91	1.38	1.25
1	A	99	GLY	CA-C	-6.90	1.39	1.52
1	A	130	PRO	C-O	6.90	1.31	1.23
1	A	97	ALA	CA-C	6.89	1.61	1.52
1	A	43	ARG	C-N	6.88	1.43	1.33
1	A	82	VAL	CA-CB	6.87	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ARG	CZ-NH2	6.85	1.42	1.33
1	A	65	GLN	CA-CB	-6.84	1.44	1.52
1	A	46	TYR	C-O	6.83	1.32	1.24
1	A	94	LEU	CB-CG	-6.82	1.39	1.53
1	A	92	GLN	N-CA	6.78	1.54	1.46
1	A	2	ALA	CA-C	6.77	1.61	1.52
1	A	107	LYS	N-CA	6.75	1.54	1.46
1	A	155	TYR	N-CA	6.75	1.54	1.46
1	A	107	LYS	CA-CB	6.73	1.65	1.53
1	A	84	ALA	N-CA	6.73	1.54	1.46
1	A	137	THR	CA-CB	6.68	1.65	1.53
1	A	65	GLN	C-O	6.59	1.31	1.23
1	A	128	MET	CA-C	6.59	1.61	1.52
1	A	31	ARG	CZ-NH2	6.57	1.42	1.33
1	A	59	ASN	CA-C	-6.57	1.44	1.52
1	A	43	ARG	NE-CZ	6.55	1.40	1.33
1	A	138	LYS	N-CA	-6.48	1.38	1.46
1	A	9	ARG	CZ-NH1	6.48	1.41	1.32
1	A	161	LYS	C-O	6.46	1.31	1.23
1	A	90	LEU	CA-CB	6.45	1.64	1.53
1	A	51	LYS	C-O	6.45	1.31	1.24
1	A	64	HIS	CD2-NE2	6.44	1.45	1.37
1	A	159	GLN	CB-CG	6.44	1.71	1.52
1	A	129	ILE	CA-C	6.43	1.59	1.52
1	A	108	ASP	CG-OD1	6.43	1.37	1.25
1	A	103	PHE	C-N	6.38	1.42	1.33
1	A	8	ASN	C-N	6.36	1.42	1.33
1	A	38	ILE	CA-CB	6.35	1.60	1.53
1	A	104	THR	N-CA	6.33	1.54	1.46
1	A	105	ALA	CA-C	-6.32	1.44	1.52
1	A	89	HIS	ND1-CE1	6.30	1.38	1.32
1	A	109	ASP	CG-OD2	6.28	1.37	1.25
1	A	24	PRO	C-N	-6.28	1.26	1.33
1	A	123	GLU	C-O	6.27	1.31	1.23
1	A	43	ARG	CA-C	6.25	1.61	1.52
1	A	55	PRO	CA-C	-6.23	1.47	1.53
1	A	121	SER	C-O	6.22	1.31	1.24
1	A	95	VAL	C-O	-6.20	1.17	1.24
1	A	127	LYS	CA-C	6.12	1.60	1.52
1	A	153	HIS	N-CA	6.11	1.53	1.45
1	A	109	ASP	CA-CB	6.11	1.62	1.53
1	A	89	HIS	CA-C	-6.10	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	HIS	ND1-CE1	6.09	1.38	1.32
1	A	87	LYS	CA-C	6.09	1.60	1.52
1	A	78	ASP	CA-C	-6.09	1.45	1.52
1	A	33	GLN	CD-NE2	-6.08	1.20	1.33
1	A	146	ASP	CG-OD2	6.06	1.36	1.25
1	A	120	GLY	N-CA	-6.05	1.38	1.45
1	A	68	TYR	CA-CB	6.05	1.63	1.53
1	A	9	ARG	CA-C	-6.05	1.44	1.52
1	A	13	ILE	CA-CB	6.03	1.62	1.54
1	A	98	GLY	C-N	5.99	1.41	1.33
1	A	119	ALA	N-CA	5.99	1.54	1.46
1	A	157	VAL	N-CA	5.93	1.54	1.46
1	A	148	ASN	N-CA	5.91	1.54	1.46
1	A	23	LEU	CB-CG	-5.90	1.41	1.53
1	A	91	ASP	CG-OD1	5.89	1.36	1.25
1	A	52	ARG	N-CA	5.88	1.60	1.45
1	A	7	GLN	C-O	-5.86	1.16	1.23
1	A	69	GLN	CD-NE2	5.86	1.45	1.33
1	A	33	GLN	CA-CB	5.84	1.63	1.53
1	A	140	SER	CB-OG	-5.84	1.30	1.42
1	A	118	LEU	N-CA	5.83	1.53	1.45
1	A	123	GLU	CD-OE1	5.83	1.36	1.25
1	A	106	PHE	CA-CB	5.81	1.62	1.53
1	A	77	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	102	ILE	CA-CB	5.80	1.62	1.54
1	A	44	ARG	CZ-NH2	5.79	1.41	1.33
1	A	83	PHE	CA-C	5.75	1.60	1.52
1	A	18	HIS	CA-CB	5.75	1.62	1.53
1	A	45	THR	N-CA	5.69	1.53	1.46
1	A	57	ARG	CZ-NH1	5.67	1.40	1.32
1	A	154	THR	CA-C	5.62	1.59	1.52
1	A	87	LYS	CD-CE	5.62	1.69	1.52
1	A	145	GLU	CG-CD	5.61	1.66	1.52
1	A	9	ARG	CA-CB	5.58	1.63	1.53
1	A	131	LEU	N-CA	5.57	1.53	1.45
1	A	145	GLU	CA-CB	5.54	1.62	1.53
1	A	36	GLY	CA-C	-5.54	1.43	1.51
1	A	133	TRP	CD2-CE2	5.54	1.50	1.41
1	A	106	PHE	N-CA	5.53	1.52	1.46
1	A	152	THR	C-N	-5.51	1.26	1.33
1	A	9	ARG	NE-CZ	5.49	1.39	1.33
1	A	113	LEU	C-O	5.49	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	LEU	N-CA	5.46	1.52	1.46
1	A	64	HIS	CG-CD2	5.46	1.41	1.35
1	A	110	VAL	N-CA	5.45	1.52	1.46
1	A	93	GLU	CD-OE1	5.44	1.35	1.25
1	A	78	ASP	CG-OD1	5.42	1.35	1.25
1	A	3	PHE	CG-CD1	5.41	1.50	1.38
1	A	9	ARG	CG-CD	5.41	1.68	1.52
1	A	22	HIS	CD2-NE2	-5.36	1.31	1.37
1	A	96	ILE	C-O	-5.36	1.18	1.24
1	A	117	ARG	CB-CG	-5.35	1.36	1.52
1	A	116	THR	CA-C	5.34	1.59	1.52
1	A	117	ARG	CA-C	5.32	1.59	1.52
1	A	15	LYS	C-O	5.32	1.30	1.23
1	A	128	MET	N-CA	5.31	1.52	1.46
1	A	78	ASP	N-CA	5.30	1.52	1.46
1	A	132	ASN	CB-CG	5.27	1.65	1.52
1	A	105	ALA	N-CA	5.27	1.53	1.46
1	A	107	LYS	CD-CE	5.27	1.68	1.52
1	A	116	THR	C-N	-5.22	1.25	1.33
1	A	153	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	26	ASP	N-CA	5.21	1.52	1.46
1	A	135	ASP	CG-OD2	5.21	1.35	1.25
1	A	61	VAL	CA-C	-5.21	1.46	1.52
1	A	93	GLU	N-CA	5.20	1.52	1.46
1	A	64	HIS	C-N	5.19	1.40	1.33
1	A	100	ALA	CA-C	5.19	1.59	1.52
1	A	135	ASP	CB-CG	5.15	1.65	1.52
1	A	31	ARG	N-CA	5.14	1.52	1.46
1	A	126	THR	CA-CB	5.14	1.62	1.53
1	A	102	ILE	N-CA	5.11	1.53	1.46
1	A	52	ARG	NE-CZ	-5.10	1.27	1.33
1	A	63	THR	C-N	-5.10	1.25	1.33
1	A	56	GLU	CB-CG	5.08	1.67	1.52
1	A	14	GLY	N-CA	5.05	1.50	1.45
1	A	36	GLY	C-O	-5.04	1.17	1.24
1	A	48	SER	C-O	-5.03	1.17	1.24
1	A	77	HIS	CG-CD2	5.01	1.41	1.35

All (510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	NE-CZ-NH2	47.11	161.60	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASN	OD1-CG-ND2	32.95	155.55	122.60
1	A	9	ARG	CD-NE-CZ	29.54	165.75	124.40
1	A	52	ARG	CA-C-O	27.58	144.82	119.72
1	A	148	ASN	CA-C-O	23.86	136.98	119.32
1	A	117	ARG	NE-CZ-NH1	-23.14	98.36	121.50
1	A	78	ASP	CA-CB-CG	22.82	135.42	112.60
1	A	52	ARG	O-C-N	-22.80	94.89	121.79
1	A	117	ARG	CD-NE-CZ	22.21	155.49	124.40
1	A	49	PHE	CA-C-N	-20.05	99.31	119.56
1	A	49	PHE	C-N-CA	-20.05	99.31	119.56
1	A	67	ASP	OD1-CG-OD2	19.23	169.06	122.90
1	A	19	LEU	CA-C-O	18.61	139.81	120.64
1	A	54	LEU	CA-C-N	-18.12	101.28	120.85
1	A	54	LEU	C-N-CA	-18.12	101.28	120.85
1	A	49	PHE	O-C-N	17.07	138.88	121.30
1	A	142	ARG	NE-CZ-NH2	-16.27	104.56	119.20
1	A	148	ASN	CA-C-N	-15.89	103.34	119.87
1	A	148	ASN	C-N-CA	-15.89	103.34	119.87
1	A	88	GLN	CA-C-O	15.88	138.91	119.38
1	A	71	GLN	OE1-CD-NE2	-15.65	106.95	122.60
1	A	54	LEU	CA-C-O	15.60	136.14	120.23
1	A	111	ASP	OD1-CG-OD2	15.57	160.26	122.90
1	A	56	GLU	OE1-CD-OE2	15.43	159.94	122.90
1	A	69	GLN	OE1-CD-NE2	-15.41	107.19	122.60
1	A	89	HIS	CA-C-O	-15.38	98.51	120.51
1	A	131	LEU	CD1-CG-CD2	15.30	144.46	110.80
1	A	34	THR	O-C-N	14.94	137.94	122.10
1	A	117	ARG	NH1-CZ-NH2	-14.85	99.99	119.30
1	A	19	LEU	CA-C-N	-14.82	104.00	120.45
1	A	19	LEU	C-N-CA	-14.82	104.00	120.45
1	A	140	SER	CA-CB-OG	-14.58	81.94	111.10
1	A	142	ARG	CD-NE-CZ	-14.54	104.05	124.40
1	A	105	ALA	O-C-N	-14.26	104.73	122.27
1	A	111	ASP	CB-CG-OD1	-14.07	86.04	118.40
1	A	64	HIS	CB-CG-CD2	-13.99	113.02	131.20
1	A	62	LEU	O-C-N	-13.86	107.42	123.22
1	A	31	ARG	NE-CZ-NH2	-13.60	106.96	119.20
1	A	10	ASN	CB-CG-OD1	-13.57	93.65	120.80
1	A	137	THR	CA-C-O	-13.51	106.39	120.71
1	A	132	ASN	CA-C-N	13.45	138.30	120.28
1	A	132	ASN	C-N-CA	13.45	138.30	120.28
1	A	26	ASP	O-C-N	-13.45	107.86	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	VAL	CA-C-O	13.45	135.39	121.67
1	A	123	GLU	O-C-N	-13.34	107.59	123.19
1	A	52	ARG	C-N-CD	13.18	149.60	120.60
1	A	159	GLN	OE1-CD-NE2	-13.13	109.47	122.60
1	A	110	VAL	CA-C-O	13.06	137.61	121.02
1	A	27	LEU	CA-C-O	-13.05	106.59	120.42
1	A	88	GLN	CA-C-N	13.02	146.41	121.54
1	A	88	GLN	C-N-CA	13.02	146.41	121.54
1	A	157	VAL	CA-C-O	-12.93	106.94	120.39
1	A	132	ASN	CA-CB-CG	-12.88	99.72	112.60
1	A	22	HIS	CA-C-O	12.65	137.48	120.15
1	A	3	PHE	CG-CD2-CE2	12.63	142.17	120.70
1	A	66	GLU	CG-CD-OE2	-12.63	89.36	118.40
1	A	110	VAL	O-C-N	-12.29	108.57	122.83
1	A	78	ASP	O-C-N	-12.18	110.48	123.26
1	A	44	ARG	N-CA-CB	-12.13	92.28	110.12
1	A	28	HIS	N-CA-C	-12.12	96.96	112.23
1	A	26	ASP	CA-C-O	12.01	133.28	120.55
1	A	132	ASN	CA-C-O	-11.93	107.70	121.66
1	A	65	GLN	CG-CD-NE2	-11.81	98.69	116.40
1	A	129	ILE	CA-C-O	11.79	135.76	119.95
1	A	54	LEU	N-CA-C	-11.76	95.35	109.93
1	A	50	PRO	CB-CA-C	-11.70	94.61	111.68
1	A	83	PHE	CA-C-O	-11.60	108.25	120.55
1	A	67	ASP	CB-CA-C	-11.60	88.07	110.11
1	A	73	ALA	O-C-N	-11.54	106.94	122.97
1	A	23	LEU	CA-C-O	11.39	134.44	121.22
1	A	66	GLU	OE1-CD-OE2	11.38	150.21	122.90
1	A	125	ASP	CA-CB-CG	11.38	123.98	112.60
1	A	89	HIS	CG-CD2-NE2	11.36	118.56	107.20
1	A	58	THR	CA-CB-OG1	-11.33	92.61	109.60
1	A	45	THR	N-CA-C	-11.25	98.99	111.14
1	A	59	ASN	O-C-N	-11.18	110.48	123.22
1	A	158	TRP	CE2-CD2-CE3	11.12	129.92	118.80
1	A	51	LYS	O-C-N	-11.11	110.08	123.30
1	A	129	ILE	CA-C-N	-11.03	108.32	119.90
1	A	129	ILE	C-N-CA	-11.03	108.32	119.90
1	A	8	ASN	CA-C-O	11.02	134.33	121.88
1	A	88	GLN	CA-CB-CG	11.02	136.14	114.10
1	A	57	ARG	NE-CZ-NH2	10.99	129.10	119.20
1	A	108	ASP	O-C-N	10.92	135.99	122.34
1	A	47	GLU	O-C-N	-10.77	108.39	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	THR	CA-C-O	-10.71	107.75	120.60
1	A	23	LEU	CA-C-N	-10.71	107.16	119.05
1	A	23	LEU	C-N-CA	-10.71	107.16	119.05
1	A	90	LEU	CA-C-O	10.69	135.79	120.51
1	A	44	ARG	NE-CZ-NH2	-10.64	109.62	119.20
1	A	45	THR	CA-C-O	-10.58	109.80	120.70
1	A	52	ARG	CB-CA-C	-10.54	96.14	110.16
1	A	159	GLN	CB-CG-CD	-10.50	94.75	112.60
1	A	80	ALA	N-CA-C	-10.49	99.84	111.28
1	A	28	HIS	CB-CG-CD2	-10.45	117.61	131.20
1	A	91	ASP	CA-CB-CG	-10.44	102.16	112.60
1	A	108	ASP	CA-C-N	-10.43	106.30	122.37
1	A	108	ASP	C-N-CA	-10.43	106.30	122.37
1	A	161	LYS	CA-C-O	-10.38	110.55	121.55
1	A	149	PRO	CA-C-N	10.35	135.19	120.28
1	A	149	PRO	C-N-CA	10.35	135.19	120.28
1	A	162	ALA	CB-CA-C	-10.26	95.11	110.50
1	A	44	ARG	CG-CD-NE	10.24	134.53	112.00
1	A	65	GLN	OE1-CD-NE2	10.21	132.81	122.60
1	A	45	THR	CA-CB-OG1	-10.19	94.32	109.60
1	A	52	ARG	CG-CD-NE	-10.19	89.58	112.00
1	A	65	GLN	O-C-N	-10.19	108.62	122.48
1	A	149	PRO	N-CA-CB	10.18	112.98	103.41
1	A	148	ASN	CB-CG-ND2	-10.14	101.19	116.40
1	A	89	HIS	ND1-CG-CD2	-10.12	95.98	106.10
1	A	56	GLU	CG-CD-OE2	-10.06	95.25	118.40
1	A	67	ASP	CB-CG-OD2	-10.06	95.26	118.40
1	A	67	ASP	N-CA-C	9.98	125.27	113.20
1	A	158	TRP	NE1-CE2-CD2	9.95	120.33	107.40
1	A	153	HIS	CG-CD2-NE2	9.94	117.14	107.20
1	A	67	ASP	CB-CG-OD1	-9.88	95.67	118.40
1	A	77	HIS	ND1-CE1-NE2	-9.76	98.64	108.40
1	A	148	ASN	N-CA-C	-9.73	95.72	109.24
1	A	123	GLU	OE1-CD-OE2	9.64	146.04	122.90
1	A	8	ASN	CB-CG-ND2	9.60	130.80	116.40
1	A	157	VAL	O-C-N	9.59	133.37	123.20
1	A	3	PHE	CD1-CG-CD2	-9.58	104.23	118.60
1	A	90	LEU	CA-C-N	9.57	139.87	122.06
1	A	90	LEU	C-N-CA	9.57	139.87	122.06
1	A	24	PRO	CA-N-CD	-9.55	98.62	112.00
1	A	107	LYS	CB-CG-CD	9.54	133.25	111.30
1	A	73	ALA	CA-C-N	9.54	136.09	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ALA	C-N-CA	9.54	136.09	123.11
1	A	28	HIS	CB-CG-ND1	9.49	136.94	122.70
1	A	13	ILE	CA-C-O	9.48	128.75	118.98
1	A	87	LYS	N-CA-CB	9.46	124.03	110.12
1	A	101	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	A	109	ASP	N-CA-CB	-9.39	95.49	110.98
1	A	21	TRP	CB-CG-CD1	9.38	140.98	126.90
1	A	9	ARG	CG-CD-NE	-9.31	91.53	112.00
1	A	161	LYS	CD-CE-NZ	9.30	141.66	111.90
1	A	123	GLU	N-CA-CB	-9.24	95.27	110.52
1	A	25	ASP	CA-C-O	9.22	130.76	120.90
1	A	105	ALA	N-CA-C	-9.22	101.13	111.82
1	A	22	HIS	CA-CB-CG	-9.21	104.59	113.80
1	A	21	TRP	CB-CG-CD2	-9.20	113.92	126.80
1	A	61	VAL	O-C-N	-9.17	113.56	123.18
1	A	8	ASN	N-CA-C	-9.12	97.77	110.35
1	A	19	LEU	N-CA-CB	9.10	122.32	110.04
1	A	20	PRO	CB-CA-C	-9.10	98.05	110.88
1	A	88	GLN	O-C-N	-9.02	110.34	122.43
1	A	62	LEU	CD1-CG-CD2	-9.01	90.98	110.80
1	A	49	PHE	CB-CG-CD1	9.01	136.01	120.70
1	A	8	ASN	OD1-CG-ND2	-8.99	113.61	122.60
1	A	132	ASN	CB-CA-C	8.98	126.23	111.41
1	A	59	ASN	CB-CG-ND2	8.94	129.80	116.40
1	A	44	ARG	O-C-N	-8.93	112.65	122.12
1	A	150	ALA	O-C-N	-8.93	111.77	122.22
1	A	90	LEU	N-CA-CB	8.93	125.58	110.49
1	A	64	HIS	CG-CD2-NE2	-8.91	98.29	107.20
1	A	118	LEU	CB-CG-CD2	-8.90	84.00	110.70
1	A	31	ARG	CD-NE-CZ	-8.89	111.95	124.40
1	A	47	GLU	CA-C-N	8.82	136.58	121.14
1	A	47	GLU	C-N-CA	8.82	136.58	121.14
1	A	149	PRO	N-CD-CG	-8.79	90.01	103.20
1	A	43	ARG	CA-C-N	-8.78	108.52	120.28
1	A	43	ARG	C-N-CA	-8.78	108.52	120.28
1	A	67	ASP	N-CA-CB	-8.72	96.29	110.42
1	A	90	LEU	O-C-N	-8.70	111.02	122.59
1	A	97	ALA	CA-C-O	-8.70	109.33	119.59
1	A	89	HIS	N-CA-CB	8.69	125.18	110.49
1	A	127	LYS	CB-CG-CD	-8.65	91.41	111.30
1	A	141	SER	O-C-N	-8.64	112.81	123.44
1	A	64	HIS	ND1-CE1-NE2	-8.63	99.77	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	HIS	CB-CG-CD2	8.62	142.41	131.20
1	A	148	ASN	CB-CG-OD1	8.54	137.87	120.80
1	A	53	PRO	CA-N-CD	-8.53	99.56	111.50
1	A	161	LYS	CG-CD-CE	-8.53	91.69	111.30
1	A	141	SER	CA-CB-OG	-8.52	94.05	111.10
1	A	46	TYR	O-C-N	-8.52	113.09	122.12
1	A	69	GLN	CG-CD-OE1	8.44	137.68	120.80
1	A	64	HIS	CB-CG-ND1	8.40	135.31	122.70
1	A	108	ASP	OD1-CG-OD2	8.40	143.07	122.90
1	A	108	ASP	CA-CB-CG	8.38	120.98	112.60
1	A	88	GLN	N-CA-C	8.37	122.75	112.54
1	A	52	ARG	CA-C-N	-8.35	106.96	127.00
1	A	52	ARG	C-N-CA	-8.35	106.96	127.00
1	A	79	VAL	CA-C-N	8.35	131.47	120.28
1	A	79	VAL	C-N-CA	8.35	131.47	120.28
1	A	55	PRO	CA-N-CD	-8.34	100.33	112.00
1	A	88	GLN	OE1-CD-NE2	-8.33	114.27	122.60
1	A	153	HIS	ND1-CG-CD2	-8.30	97.80	106.10
1	A	101	GLN	CA-CB-CG	-8.28	97.54	114.10
1	A	50	PRO	CA-C-N	8.26	134.64	122.99
1	A	50	PRO	C-N-CA	8.26	134.64	122.99
1	A	62	LEU	N-CA-CB	8.26	123.89	110.42
1	A	57	ARG	N-CA-C	-8.23	96.20	108.79
1	A	78	ASP	OD1-CG-OD2	8.16	142.48	122.90
1	A	123	GLU	CA-C-O	8.14	129.83	120.80
1	A	66	GLU	CA-CB-CG	-8.13	97.84	114.10
1	A	88	GLN	CG-CD-OE1	8.12	137.04	120.80
1	A	91	ASP	OD1-CG-OD2	-8.11	103.43	122.90
1	A	145	GLU	CB-CG-CD	-8.10	98.83	112.60
1	A	30	PHE	O-C-N	8.08	130.50	122.09
1	A	113	LEU	CA-C-O	-8.03	111.48	120.32
1	A	144	VAL	CA-C-N	-8.03	110.68	122.65
1	A	144	VAL	C-N-CA	-8.03	110.68	122.65
1	A	34	THR	CA-C-N	-8.00	109.78	120.50
1	A	34	THR	C-N-CA	-8.00	109.78	120.50
1	A	33	GLN	CG-CD-NE2	-7.99	104.41	116.40
1	A	137	THR	CA-CB-OG1	-7.98	97.63	109.60
1	A	82	VAL	O-C-N	-7.96	113.42	121.94
1	A	97	ALA	O-C-N	7.94	131.70	122.25
1	A	126	THR	CA-CB-OG1	-7.94	97.69	109.60
1	A	117	ARG	CA-C-O	-7.94	111.87	120.36
1	A	47	GLU	CA-CB-CG	-7.91	98.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLN	CB-CG-CD	7.85	125.94	112.60
1	A	42	GLY	CA-C-O	7.83	130.35	121.90
1	A	92	GLN	CA-C-O	7.77	128.85	120.38
1	A	142	ARG	NH1-CZ-NH2	7.76	129.40	119.30
1	A	89	HIS	CB-CA-C	7.74	125.82	110.42
1	A	5	TRP	CE3-CZ3-CH2	7.71	131.12	121.10
1	A	74	VAL	CA-C-O	7.67	129.64	120.66
1	A	49	PHE	CB-CG-CD2	-7.67	107.67	120.70
1	A	161	LYS	CB-CG-CD	-7.66	93.69	111.30
1	A	149	PRO	CA-CB-CG	-7.63	90.00	104.50
1	A	82	VAL	CA-C-O	7.61	130.01	121.18
1	A	90	LEU	CA-CB-CG	-7.58	89.78	116.30
1	A	123	GLU	CG-CD-OE2	-7.58	100.98	118.40
1	A	69	GLN	CA-C-O	7.57	128.53	120.36
1	A	122	PHE	CA-CB-CG	-7.55	106.25	113.80
1	A	124	GLY	CA-C-O	7.53	129.27	121.21
1	A	135	ASP	N-CA-CB	7.51	122.59	110.42
1	A	98	GLY	CA-C-O	-7.49	114.85	122.56
1	A	89	HIS	CE1-NE2-CD2	-7.44	101.56	109.00
1	A	50	PRO	CA-N-CD	-7.44	101.59	112.00
1	A	49	PHE	C-N-CD	7.39	155.30	125.00
1	A	50	PRO	N-CD-CG	-7.38	92.13	103.20
1	A	68	TYR	CB-CG-CD1	-7.38	109.73	120.80
1	A	74	VAL	O-C-N	-7.32	113.29	122.88
1	A	135	ASP	OD1-CG-OD2	7.28	140.38	122.90
1	A	91	ASP	CB-CG-OD1	7.27	135.11	118.40
1	A	20	PRO	CA-N-CD	-7.25	101.85	112.00
1	A	64	HIS	CA-CB-CG	-7.23	106.57	113.80
1	A	62	LEU	CB-CG-CD2	-7.23	89.02	110.70
1	A	155	TYR	CB-CG-CD1	-7.15	110.07	120.80
1	A	109	ASP	CB-CG-OD2	-7.14	101.97	118.40
1	A	118	LEU	CB-CA-C	7.14	121.72	109.51
1	A	134	ASP	CB-CG-OD2	-7.13	102.00	118.40
1	A	125	ASP	CB-CG-OD2	7.13	134.79	118.40
1	A	84	ALA	O-C-N	-7.09	114.60	122.12
1	A	135	ASP	CB-CG-OD2	-7.09	102.09	118.40
1	A	87	LYS	O-C-N	-7.09	114.60	122.12
1	A	128	MET	CA-C-O	7.07	129.08	121.16
1	A	92	GLN	CB-CG-CD	-7.07	100.58	112.60
1	A	107	LYS	N-CA-C	-7.07	103.76	112.38
1	A	5	TRP	CZ3-CH2-CZ2	-7.06	112.32	121.50
1	A	142	ARG	N-CA-C	-7.04	96.22	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	LEU	C-N-CD	7.04	153.88	125.00
1	A	83	PHE	CB-CG-CD2	-7.04	108.73	120.70
1	A	145	GLU	CA-C-O	7.01	128.58	120.80
1	A	34	THR	CA-C-O	-7.01	110.56	118.55
1	A	117	ARG	O-C-N	6.99	131.19	123.22
1	A	150	ALA	CA-C-N	6.98	133.94	121.66
1	A	150	ALA	C-N-CA	6.98	133.94	121.66
1	A	82	VAL	N-CA-C	-6.94	103.90	110.42
1	A	78	ASP	N-CA-CB	-6.93	100.79	111.46
1	A	18	HIS	CA-CB-CG	6.92	120.72	113.80
1	A	24	PRO	CA-C-O	-6.91	109.09	119.86
1	A	29	TYR	CG-CD2-CE2	6.87	131.51	121.20
1	A	54	LEU	C-N-CD	6.87	153.16	125.00
1	A	105	ALA	CA-C-N	6.86	133.31	122.60
1	A	105	ALA	C-N-CA	6.86	133.31	122.60
1	A	125	ASP	N-CA-CB	-6.83	100.35	111.01
1	A	105	ALA	CA-C-O	-6.83	112.12	119.97
1	A	153	HIS	CE1-NE2-CD2	-6.83	102.17	109.00
1	A	145	GLU	O-C-N	-6.81	115.22	123.19
1	A	132	ASN	CB-CG-ND2	-6.80	106.20	116.40
1	A	41	VAL	CA-C-N	6.80	126.80	120.34
1	A	41	VAL	C-N-CA	6.80	126.80	120.34
1	A	109	ASP	N-CA-C	-6.79	103.36	112.94
1	A	158	TRP	CE2-CD2-CG	-6.77	99.08	107.20
1	A	28	HIS	CA-C-O	-6.76	111.81	119.79
1	A	159	GLN	CG-CD-OE1	6.74	134.28	120.80
1	A	13	ILE	CA-C-N	-6.74	110.08	121.47
1	A	13	ILE	C-N-CA	-6.74	110.08	121.47
1	A	64	HIS	O-C-N	6.74	131.98	122.41
1	A	42	GLY	O-C-N	-6.72	114.22	122.76
1	A	134	ASP	O-C-N	-6.72	114.00	122.27
1	A	102	ILE	CA-CB-CG2	6.72	121.92	110.50
1	A	19	LEU	C-N-CD	6.71	152.50	125.00
1	A	27	LEU	O-C-N	6.71	129.79	122.15
1	A	109	ASP	OD1-CG-OD2	6.68	138.94	122.90
1	A	150	ALA	CA-C-O	6.68	127.65	120.10
1	A	104	THR	N-CA-CB	-6.68	100.31	110.12
1	A	121	SER	N-CA-CB	-6.67	99.48	110.68
1	A	95	VAL	O-C-N	6.63	130.23	123.20
1	A	7	GLN	CA-C-O	6.62	128.74	121.06
1	A	130	PRO	N-CA-CB	6.61	109.17	103.36
1	A	151	LEU	N-CA-CB	6.59	120.73	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ILE	N-CA-C	6.59	119.99	113.53
1	A	80	ALA	CA-C-O	-6.58	113.57	120.55
1	A	20	PRO	CA-C-N	6.58	133.12	122.53
1	A	20	PRO	C-N-CA	6.58	133.12	122.53
1	A	99	GLY	O-C-N	-6.57	112.50	123.00
1	A	19	LEU	N-CA-C	-6.56	100.66	110.24
1	A	55	PRO	CB-CA-C	-6.55	100.64	110.20
1	A	96	ILE	CA-CB-CG1	6.54	121.52	110.40
1	A	44	ARG	N-CA-C	6.54	118.41	111.28
1	A	148	ASN	C-N-CD	6.53	151.75	125.00
1	A	109	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	135	ASP	O-C-N	6.52	132.03	122.39
1	A	48	SER	CA-C-O	6.50	127.38	119.31
1	A	23	LEU	N-CA-CB	6.50	119.15	111.09
1	A	78	ASP	CB-CA-C	6.49	123.90	111.17
1	A	93	GLU	CG-CD-OE1	-6.49	103.48	118.40
1	A	67	ASP	CA-C-O	6.48	127.61	119.12
1	A	53	PRO	CB-CG-CD	-6.48	90.49	105.40
1	A	63	THR	OG1-CB-CG2	6.47	122.23	109.30
1	A	33	GLN	CA-C-N	-6.45	112.21	122.08
1	A	33	GLN	C-N-CA	-6.45	112.21	122.08
1	A	30	PHE	CA-C-N	-6.44	112.07	120.44
1	A	30	PHE	C-N-CA	-6.44	112.07	120.44
1	A	134	ASP	N-CA-C	-6.43	104.36	111.82
1	A	32	ALA	CA-C-O	6.43	127.57	120.63
1	A	64	HIS	CE1-NE2-CD2	6.41	115.41	109.00
1	A	1	THR	CA-CB-CG2	6.39	121.36	110.50
1	A	83	PHE	CE1-CZ-CE2	6.39	131.50	120.00
1	A	35	VAL	CA-CB-CG1	-6.38	99.55	110.40
1	A	119	ALA	N-CA-CB	-6.38	99.99	110.40
1	A	161	LYS	O-C-N	-6.38	114.97	122.81
1	A	25	ASP	OD1-CG-OD2	-6.37	107.61	122.90
1	A	1	THR	OG1-CB-CG2	-6.35	96.59	109.30
1	A	106	PHE	N-CA-C	-6.35	104.68	112.88
1	A	33	GLN	CA-C-O	-6.33	111.01	119.11
1	A	142	ARG	CG-CD-NE	6.32	125.91	112.00
1	A	91	ASP	N-CA-C	-6.32	105.57	113.28
1	A	111	ASP	CB-CA-C	6.32	119.69	109.07
1	A	44	ARG	CB-CG-CD	-6.31	96.79	111.30
1	A	153	HIS	ND1-CE1-NE2	6.30	114.70	108.40
1	A	57	ARG	CB-CG-CD	-6.30	96.81	111.30
1	A	159	GLN	CA-C-O	6.29	127.90	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ARG	N-CA-C	-6.29	88.75	107.37
1	A	18	HIS	CE1-NE2-CD2	-6.29	102.71	109.00
1	A	96	ILE	CA-CB-CG2	-6.27	99.83	110.50
1	A	158	TRP	CD2-CE2-CZ2	-6.26	116.14	122.40
1	A	145	GLU	CG-CD-OE1	-6.25	104.01	118.40
1	A	71	GLN	CA-CB-CG	-6.25	101.59	114.10
1	A	144	VAL	CA-CB-CG2	-6.25	99.78	110.40
1	A	75	VAL	N-CA-CB	6.25	119.22	111.41
1	A	12	LEU	O-C-N	-6.24	115.19	122.87
1	A	119	ALA	O-C-N	-6.24	113.85	122.46
1	A	83	PHE	CD1-CE1-CZ	-6.23	108.78	120.00
1	A	106	PHE	CB-CG-CD1	6.23	131.29	120.70
1	A	108	ASP	CB-CG-OD2	-6.22	104.09	118.40
1	A	118	LEU	CD1-CG-CD2	-6.22	97.11	110.80
1	A	25	ASP	CB-CG-OD1	6.22	132.70	118.40
1	A	51	LYS	N-CA-C	-6.18	98.82	108.90
1	A	56	GLU	CG-CD-OE1	-6.18	104.18	118.40
1	A	141	SER	N-CA-CB	-6.16	100.48	110.71
1	A	59	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	A	29	TYR	CD1-CG-CD2	-6.15	108.88	118.10
1	A	34	THR	N-CA-C	-6.11	106.80	114.56
1	A	93	GLU	CA-CB-CG	6.11	126.31	114.10
1	A	15	LYS	CB-CA-C	-6.10	101.33	110.24
1	A	136	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	58	THR	O-C-N	6.09	130.13	123.13
1	A	11	GLY	CA-C-N	-6.07	112.10	120.71
1	A	11	GLY	C-N-CA	-6.07	112.10	120.71
1	A	37	LYS	N-CA-CB	-6.05	101.41	110.60
1	A	38	ILE	O-C-N	-6.03	115.29	122.77
1	A	20	PRO	O-C-N	-6.03	112.48	122.36
1	A	123	GLU	CA-C-N	6.02	128.94	120.57
1	A	123	GLU	C-N-CA	6.02	128.94	120.57
1	A	99	GLY	CA-C-N	6.01	128.62	120.38
1	A	99	GLY	C-N-CA	6.01	128.62	120.38
1	A	119	ALA	N-CA-C	-6.01	105.43	112.89
1	A	134	ASP	CA-C-N	5.96	133.86	121.94
1	A	134	ASP	C-N-CA	5.96	133.86	121.94
1	A	29	TYR	CB-CG-CD2	5.94	129.71	120.80
1	A	9	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	A	31	ARG	NE-CZ-NH1	5.94	127.44	121.50
1	A	130	PRO	CA-N-CD	-5.91	103.72	112.00
1	A	15	LYS	O-C-N	-5.90	115.26	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	85	TYR	O-C-N	-5.88	115.74	122.09
1	A	107	LYS	CA-C-O	-5.87	112.39	119.49
1	A	108	ASP	CA-C-O	-5.87	112.48	119.35
1	A	9	ARG	N-CA-C	5.86	119.53	112.38
1	A	59	ASN	CA-C-O	5.86	126.63	120.36
1	A	65	GLN	CA-C-N	5.86	132.73	121.54
1	A	65	GLN	C-N-CA	5.86	132.73	121.54
1	A	74	VAL	N-CA-C	-5.82	98.76	107.37
1	A	39	MET	CA-C-O	-5.82	114.36	120.58
1	A	3	PHE	CB-CG-CD1	5.81	130.58	120.70
1	A	31	ARG	CG-CD-NE	5.80	124.76	112.00
1	A	109	ASP	O-C-N	-5.79	115.18	122.19
1	A	142	ARG	CA-CB-CG	-5.79	102.52	114.10
1	A	143	THR	O-C-N	-5.75	116.50	123.29
1	A	8	ASN	CB-CA-C	5.74	124.52	111.71
1	A	40	VAL	O-C-N	5.71	129.37	123.03
1	A	57	ARG	NH1-CZ-NH2	-5.71	111.87	119.30
1	A	86	ALA	CA-C-N	5.70	127.92	120.28
1	A	86	ALA	C-N-CA	5.70	127.92	120.28
1	A	38	ILE	CB-CG1-CD1	-5.69	101.86	113.80
1	A	121	SER	O-C-N	-5.68	116.54	123.30
1	A	92	GLN	CA-CB-CG	-5.67	102.77	114.10
1	A	71	GLN	CB-CG-CD	-5.66	102.98	112.60
1	A	77	HIS	ND1-CG-CD2	-5.66	100.44	106.10
1	A	21	TRP	CA-C-O	5.64	127.66	121.40
1	A	66	GLU	CA-C-O	5.63	128.56	120.51
1	A	154	THR	CA-CB-OG1	-5.62	101.18	109.60
1	A	22	HIS	CB-CG-ND1	5.61	131.12	122.70
1	A	83	PHE	CD1-CG-CD2	5.61	127.01	118.60
1	A	149	PRO	CB-CA-C	-5.61	102.97	111.44
1	A	130	PRO	CA-C-O	-5.59	114.66	121.03
1	A	91	ASP	CA-C-N	-5.59	115.29	123.00
1	A	91	ASP	C-N-CA	-5.59	115.29	123.00
1	A	78	ASP	CB-CG-OD2	-5.58	105.56	118.40
1	A	75	VAL	O-C-N	-5.58	114.55	122.76
1	A	135	ASP	CB-CA-C	-5.58	99.50	110.11
1	A	96	ILE	CB-CA-C	5.57	118.61	110.98
1	A	106	PHE	CG-CD1-CE1	5.56	130.15	120.70
1	A	106	PHE	CD1-CE1-CZ	-5.55	110.01	120.00
1	A	23	LEU	O-C-N	5.55	125.89	121.17
1	A	75	VAL	CA-C-N	5.54	130.90	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	C-N-CA	5.54	130.90	122.92
1	A	72	GLY	CA-C-O	-5.54	113.17	119.04
1	A	64	HIS	ND1-CG-CD2	5.54	111.64	106.10
1	A	85	TYR	CA-C-N	5.54	127.96	120.38
1	A	85	TYR	C-N-CA	5.54	127.96	120.38
1	A	107	LYS	CD-CE-NZ	-5.54	94.19	111.90
1	A	61	VAL	CA-C-O	5.53	126.34	120.48
1	A	130	PRO	N-CA-C	5.51	119.12	110.80
1	A	37	LYS	CA-CB-CG	-5.49	103.11	114.10
1	A	52	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	31	ARG	O-C-N	-5.49	116.42	122.07
1	A	10	ASN	CA-CB-CG	-5.47	107.13	112.60
1	A	104	THR	OG1-CB-CG2	-5.46	98.38	109.30
1	A	129	ILE	C-N-CD	5.46	147.40	125.00
1	A	60	VAL	N-CA-CB	-5.46	104.59	111.46
1	A	28	HIS	O-C-N	-5.45	115.03	122.33
1	A	101	GLN	CB-CA-C	-5.43	101.61	110.85
1	A	106	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	78	ASP	CA-C-N	5.43	129.21	120.30
1	A	78	ASP	C-N-CA	5.43	129.21	120.30
1	A	159	GLN	CA-C-N	5.42	129.04	121.02
1	A	159	GLN	C-N-CA	5.42	129.04	121.02
1	A	91	ASP	CB-CA-C	5.42	120.12	109.72
1	A	37	LYS	CD-CE-NZ	5.41	129.22	111.90
1	A	133	TRP	N-CA-C	-5.41	105.38	111.28
1	A	102	ILE	CG1-CB-CG2	-5.39	94.53	110.70
1	A	24	PRO	CA-CB-CG	-5.38	94.27	104.50
1	A	144	VAL	N-CA-CB	5.38	118.64	111.64
1	A	83	PHE	O-C-N	5.38	127.83	122.12
1	A	98	GLY	N-CA-C	5.38	119.70	112.17
1	A	112	THR	N-CA-CB	-5.38	101.51	111.13
1	A	125	ASP	OD1-CG-OD2	-5.38	110.00	122.90
1	A	22	HIS	ND1-CE1-NE2	-5.36	103.04	108.40
1	A	103	PHE	CG-CD1-CE1	-5.36	111.59	120.70
1	A	94	LEU	CA-C-O	5.36	126.09	120.36
1	A	11	GLY	CA-C-O	5.35	124.95	119.01
1	A	118	LEU	N-CA-C	-5.34	101.83	110.32
1	A	21	TRP	O-C-N	-5.34	115.68	122.78
1	A	66	GLU	O-C-N	-5.33	115.50	122.59
1	A	89	HIS	CA-C-N	-5.32	111.37	121.54
1	A	89	HIS	C-N-CA	-5.32	111.37	121.54
1	A	63	THR	O-C-N	-5.31	116.91	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ILE	CA-CB-CG1	5.30	119.41	110.40
1	A	82	VAL	N-CA-CB	5.30	116.64	110.65
1	A	151	LEU	CA-C-O	5.30	125.47	119.27
1	A	92	GLN	N-CA-C	-5.29	100.54	109.07
1	A	47	GLU	CB-CG-CD	-5.29	103.61	112.60
1	A	84	ALA	N-CA-C	-5.29	105.52	111.28
1	A	131	LEU	N-CA-C	-5.28	101.33	109.52
1	A	146	ASP	CA-C-O	-5.28	115.14	121.11
1	A	16	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	102	ILE	O-C-N	5.27	127.76	121.80
1	A	10	ASN	CA-C-O	-5.27	113.19	119.35
1	A	150	ALA	N-CA-C	-5.27	105.66	111.71
1	A	63	THR	CA-CB-OG1	-5.24	101.73	109.60
1	A	92	GLN	O-C-N	-5.24	117.10	123.29
1	A	151	LEU	CD1-CG-CD2	5.23	122.31	110.80
1	A	58	THR	CA-C-O	-5.22	114.58	120.43
1	A	24	PRO	CA-C-N	5.22	127.58	120.54
1	A	24	PRO	C-N-CA	5.22	127.58	120.54
1	A	103	PHE	CD1-CG-CD2	5.22	126.42	118.60
1	A	71	GLN	CG-CD-OE1	5.21	131.22	120.80
1	A	90	LEU	CB-CG-CD1	5.21	126.34	110.70
1	A	93	GLU	O-C-N	-5.21	116.54	122.89
1	A	43	ARG	O-C-N	5.21	127.50	122.09
1	A	156	GLU	CB-CG-CD	-5.18	103.79	112.60
1	A	93	GLU	CB-CG-CD	-5.17	103.80	112.60
1	A	47	GLU	CA-C-O	5.15	125.72	119.49
1	A	88	GLN	CG-CD-NE2	-5.14	108.69	116.40
1	A	149	PRO	CA-N-CD	-5.13	104.81	112.00
1	A	90	LEU	CB-CA-C	5.13	120.63	110.42
1	A	130	PRO	CA-C-N	-5.12	114.55	122.59
1	A	130	PRO	C-N-CA	-5.12	114.55	122.59
1	A	135	ASP	CA-C-N	-5.10	114.58	122.59
1	A	135	ASP	C-N-CA	-5.10	114.58	122.59
1	A	161	LYS	N-CA-CB	-5.08	102.57	110.04
1	A	134	ASP	CB-CG-OD1	5.08	130.07	118.40
1	A	43	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	A	146	ASP	CB-CG-OD1	5.06	130.05	118.40
1	A	100	ALA	N-CA-C	5.06	117.45	111.33
1	A	83	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	3	PHE	CE1-CZ-CE2	-5.05	110.90	120.00
1	A	38	ILE	CA-C-N	5.05	129.14	122.42
1	A	38	ILE	C-N-CA	5.05	129.14	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	VAL	O-C-N	5.02	127.96	122.63
1	A	42	GLY	N-CA-C	-5.01	105.68	112.14
1	A	77	HIS	CG-ND1-CE1	5.01	117.82	109.30
1	A	44	ARG	CA-C-N	5.01	127.25	120.44
1	A	44	ARG	C-N-CA	5.01	127.25	120.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	89	HIS	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Mainchain
1	A	21	TRP	Mainchain
1	A	31	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	57	ARG	Sidechain
1	A	78	ASP	Mainchain
1	A	9	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	1294	0	1256	32	0
2	A	48	0	26	0	0
3	A	33	0	20	1	0
4	A	264	0	0	1	0
All	All	1639	0	1302	32	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 (32) 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:A:145:GLU:CB	1:A:145:GLU:CG	1.77	1.58
1:A:90:LEU:CG	1:A:90:LEU:CD1	1.88	1.50
1:A:67:ASP:CA	1:A:67:ASP:CB	1.87	1.48
1:A:90:LEU:CG	1:A:90:LEU:CD2	1.94	1.44
1:A:50:PRO:N	1:A:50:PRO:CD	1.78	1.38
1:A:149:PRO:N	1:A:149:PRO:CD	1.70	1.37
1:A:55:PRO:N	1:A:55:PRO:CD	1.69	1.35
1:A:130:PRO:N	1:A:130:PRO:CD	1.73	1.33
1:A:53:PRO:CD	1:A:53:PRO:N	1.68	1.33
1:A:24:PRO:CD	1:A:24:PRO:N	1.78	1.29
1:A:67:ASP:CB	1:A:67:ASP:C	2.34	0.99
1:A:90:LEU:CD2	1:A:90:LEU:CB	2.60	0.78
1:A:89:HIS:O	1:A:90:LEU:HB2	1.83	0.77
1:A:67:ASP:CB	1:A:67:ASP:N	2.49	0.76
1:A:145:GLU:CB	1:A:145:GLU:CD	2.60	0.74
1:A:89:HIS:O	1:A:90:LEU:CB	2.37	0.73
1:A:67:ASP:CA	1:A:67:ASP:CG	2.69	0.63
1:A:8:ASN:ND2	1:A:12:LEU:H	1.96	0.62
1:A:145:GLU:CG	1:A:145:GLU:CA	2.83	0.52
1:A:19:LEU:HD11	3:A:164:MTX:H7	1.92	0.51
1:A:67:ASP:CB	1:A:67:ASP:H	2.23	0.49
1:A:18:HIS:HB3	4:A:403:HOH:O	2.13	0.47
1:A:15:LYS:HG3	1:A:124:GLY:HA2	1.97	0.46
1:A:67:ASP:CA	1:A:67:ASP:OD1	2.62	0.46
1:A:87:LYS:O	1:A:90:LEU:HD12	2.15	0.46
1:A:67:ASP:CG	1:A:67:ASP:H	2.24	0.46
1:A:23:LEU:O	1:A:24:PRO:C	2.60	0.44
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.92	0.43
1:A:67:ASP:N	1:A:67:ASP:CG	2.78	0.41
1:A:107:LYS:HE3	1:A:130:PRO:O	2.20	0.41
1:A:41:VAL:HG11	1:A:49:PHE:HZ	1.85	0.41
1:A:142:ARG:HH11	1:A:142:ARG:HD2	1.74	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	21 9

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LEU

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	136/137 (99%)	127 (93%)	9 (7%)	15 4

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ARG
1	A	24	PRO
1	A	87	LYS
1	A	88	GLN
1	A	89	HIS
1	A	90	LEU
1	A	102	ILE
1	A	111	ASP

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	33	GLN
1	A	92	GLN
1	A	101	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	164	-	35,35,35	3.48	12 (34%)	47,49,49	5.41	32 (68%)
2	NDP	A	163	-	51,52,52	2.32	21 (41%)	71,80,80	2.94	30 (42%)

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	164	-	-	6/25/25/25	0/3/3/3
2	NDP	A	163	-	-	3/34/77/77	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	164	MTX	C11-C	-8.85	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	164	MTX	C13-C14	8.48	1.55	1.39
3	A	164	MTX	CG-CD	7.19	1.67	1.50
3	A	164	MTX	C16-C15	-6.26	1.28	1.38
2	A	163	NDP	C5A-C6A	6.16	1.58	1.41
3	A	164	MTX	C7-N8	-6.16	1.21	1.31
2	A	163	NDP	O4B-C4B	-5.89	1.31	1.45
3	A	164	MTX	C15-C14	5.49	1.49	1.39
3	A	164	MTX	OE1-CD	4.65	1.37	1.22
3	A	164	MTX	CA-N	-4.54	1.36	1.45
2	A	163	NDP	P2B-O2B	4.50	1.67	1.59
3	A	164	MTX	C9-N10	-4.08	1.38	1.46
2	A	163	NDP	C4A-N3A	3.96	1.41	1.34
3	A	164	MTX	CM-N10	3.92	1.52	1.46
2	A	163	NDP	C6N-N1N	3.55	1.45	1.37
2	A	163	NDP	C2A-N1A	3.50	1.40	1.33
2	A	163	NDP	C3B-C2B	3.23	1.60	1.53
2	A	163	NDP	C6A-N1A	-3.23	1.26	1.35
2	A	163	NDP	O7N-C7N	3.19	1.31	1.24
2	A	163	NDP	C5B-C4B	2.96	1.60	1.51
2	A	163	NDP	O4B-C1B	2.82	1.48	1.42
2	A	163	NDP	C1D-N1N	2.73	1.53	1.46
2	A	163	NDP	C3B-C4B	2.57	1.59	1.53
2	A	163	NDP	C8A-N7A	-2.55	1.26	1.31
2	A	163	NDP	C5A-N7A	2.54	1.43	1.39
3	A	164	MTX	O2-CT	2.40	1.38	1.30
2	A	163	NDP	O3B-C3B	2.28	1.48	1.43
2	A	163	NDP	C7N-C3N	-2.24	1.43	1.48
2	A	163	NDP	C2N-C3N	-2.18	1.29	1.35
2	A	163	NDP	C6N-C5N	2.12	1.39	1.33
3	A	164	MTX	C13-C12	-2.11	1.35	1.38
2	A	163	NDP	O4D-C4D	2.07	1.49	1.45
2	A	163	NDP	PN-O1N	-2.00	1.43	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	MTX	O-C-N	-14.81	94.31	122.47
3	A	164	MTX	C9-N10-C14	10.68	133.11	120.17
3	A	164	MTX	C13-C12-C11	10.00	131.48	120.80
2	A	163	NDP	O7N-C7N-C3N	-9.68	102.66	120.90
3	A	164	MTX	CA-N-C	9.25	143.75	121.56
3	A	164	MTX	OE2-CD-CG	-9.21	84.90	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	MTX	OE2-CD-OE1	9.20	146.99	123.33
3	A	164	MTX	CB-CG-CD	8.60	135.44	112.49
3	A	164	MTX	C12-C13-C14	-8.60	109.42	120.30
3	A	164	MTX	C6-C7-N8	8.30	131.10	123.14
3	A	164	MTX	O-C-C11	8.19	137.13	120.90
3	A	164	MTX	CB-CA-N	7.55	125.85	110.91
3	A	164	MTX	C4A-C4-N3	-7.32	112.17	120.84
2	A	163	NDP	C3N-C7N-N7N	6.71	129.59	117.67
2	A	163	NDP	C4A-N9A-C8A	-6.17	99.26	105.74
3	A	164	MTX	C11-C-N	5.81	127.81	117.04
2	A	163	NDP	O2X-P2B-O1X	5.59	132.60	110.83
2	A	163	NDP	C1D-N1N-C2N	5.45	130.12	121.14
2	A	163	NDP	C2B-C3B-C4B	-5.41	90.35	101.99
2	A	163	NDP	C1D-N1N-C6N	-5.21	109.75	120.77
2	A	163	NDP	C5A-C4A-N9A	5.17	111.45	105.81
2	A	163	NDP	N9A-C8A-N7A	5.07	121.13	113.94
3	A	164	MTX	CB-CA-CT	-4.89	98.74	110.35
3	A	164	MTX	N1-C2-N3	-4.73	121.20	127.21
2	A	163	NDP	N6A-C6A-N1A	4.59	128.61	118.38
3	A	164	MTX	C16-C15-C14	4.34	125.79	120.30
3	A	164	MTX	C7-C6-N5	-4.08	118.22	120.87
3	A	164	MTX	NA2-C2-N3	3.91	123.09	117.22
2	A	163	NDP	O4B-C1B-C2B	-3.89	99.89	106.59
2	A	163	NDP	C4A-C5A-N7A	-3.85	106.18	110.58
3	A	164	MTX	CG-CB-CA	3.81	120.19	113.16
2	A	163	NDP	O2N-PN-O1N	3.79	130.07	112.44
3	A	164	MTX	C7-N8-C8A	-3.77	111.94	117.20
2	A	163	NDP	N3A-C4A-N9A	-3.77	120.76	127.17
3	A	164	MTX	O1-CT-CA	3.75	134.34	122.26
3	A	164	MTX	C2-N3-C4	3.75	127.41	116.72
2	A	163	NDP	N3A-C2A-N1A	3.69	134.16	128.58
2	A	163	NDP	O3B-C3B-C4B	-3.63	100.67	111.08
2	A	163	NDP	C2A-N3A-C4A	-3.60	103.04	111.83
3	A	164	MTX	C15-C14-N10	-3.56	116.62	121.59
3	A	164	MTX	C9-C6-C7	3.46	127.68	121.38
2	A	163	NDP	O4D-C1D-N1N	3.45	114.66	108.08
2	A	163	NDP	C5A-C6A-N1A	-3.42	108.82	117.51
3	A	164	MTX	C13-C14-N10	3.32	126.22	121.59
2	A	163	NDP	O4B-C4B-C5B	-3.31	98.74	109.33
3	A	164	MTX	NA4-C4-N3	3.17	125.62	117.11
2	A	163	NDP	O3B-C3B-C2B	3.17	120.05	111.19
2	A	163	NDP	C5B-C4B-C3B	-3.10	104.05	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	MTX	O2-CT-O1	-3.08	117.09	124.08
3	A	164	MTX	C15-C16-C11	-3.02	117.57	120.80
2	A	163	NDP	C2A-N1A-C6A	3.00	123.66	118.73
2	A	163	NDP	C6A-C5A-C4A	2.91	121.16	117.18
3	A	164	MTX	CM-N10-C14	-2.90	114.79	119.59
2	A	163	NDP	O2B-P2B-O1X	-2.54	100.27	109.33
2	A	163	NDP	C1B-N9A-C8A	2.44	132.52	127.09
3	A	164	MTX	C9-C6-N5	-2.40	113.20	117.09
2	A	163	NDP	C5A-N7A-C8A	-2.34	99.78	103.45
2	A	163	NDP	C3N-C2N-N1N	2.24	126.49	123.20
2	A	163	NDP	O2N-PN-O5D	-2.20	97.60	107.57
2	A	163	NDP	O3X-P2B-O2B	-2.13	97.56	105.85
3	A	164	MTX	C8A-C4A-N5	-2.04	120.07	122.35
3	A	164	MTX	C12-C11-C	-2.00	114.11	120.60

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	164	MTX	O-C-N-CA
2	A	163	NDP	O4D-C1D-N1N-C2N
3	A	164	MTX	CA-CB-CG-CD
3	A	164	MTX	C11-C-N-CA
2	A	163	NDP	C2B-O2B-P2B-O3X
3	A	164	MTX	C6-C9-N10-CM
3	A	164	MTX	OE2-CD-CG-CB
3	A	164	MTX	OE1-CD-CG-CB
2	A	163	NDP	PN-O3-PA-O2A

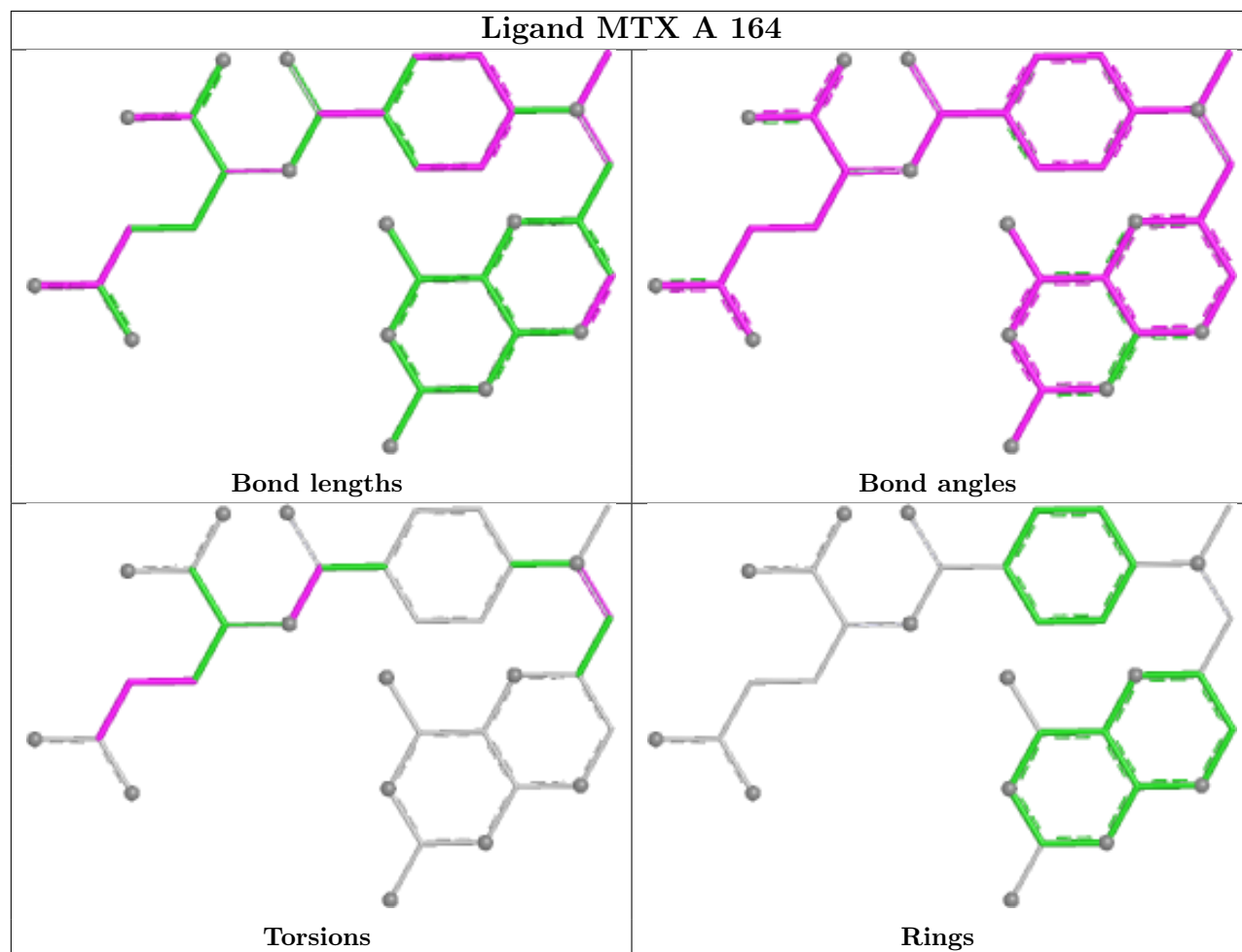
There are no ring outliers.

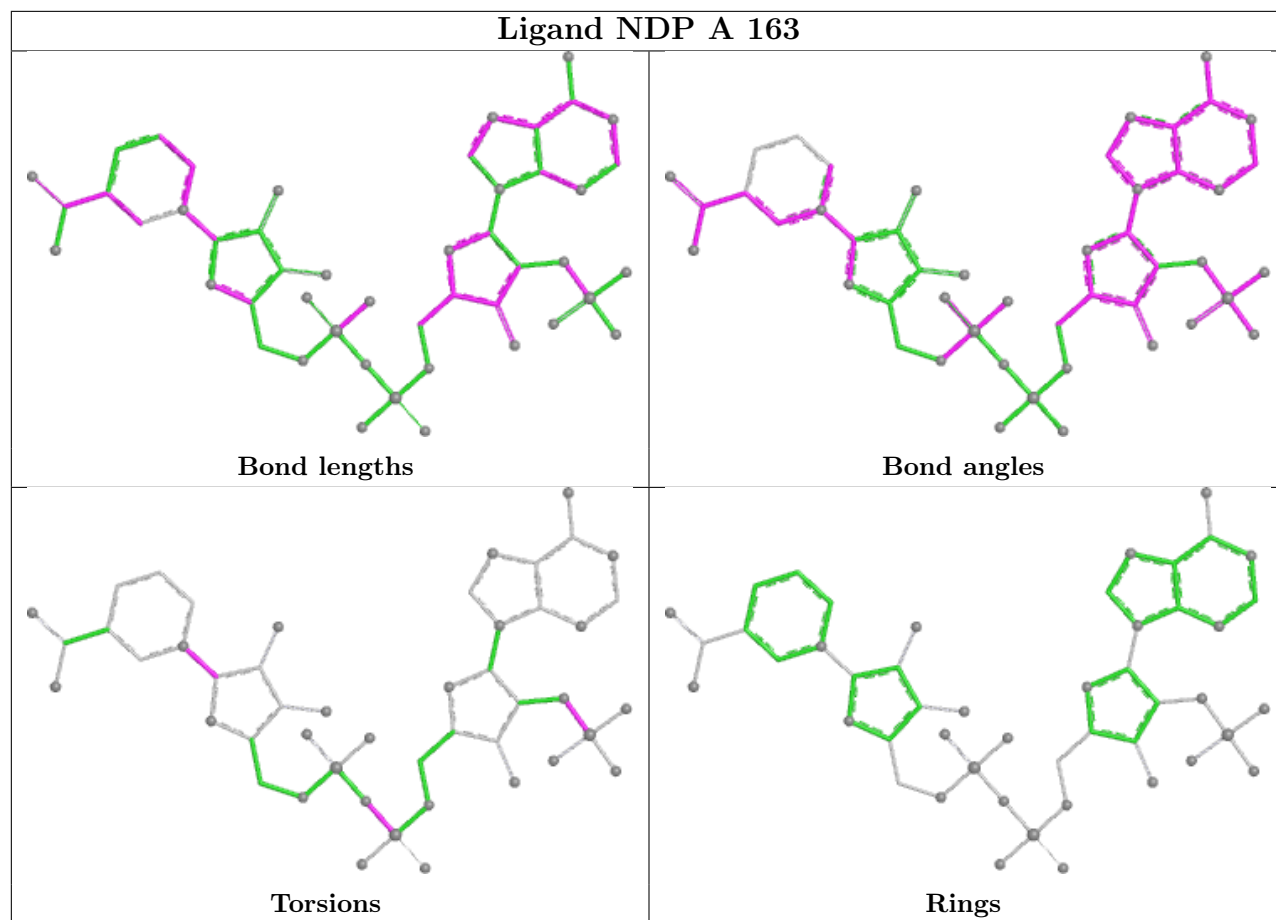
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	164	MTX	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:ARG	C	53:PRO	N	1.64
1	A	89:HIS	C	90:LEU	N	0.96

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.