



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:57 am BST

PDB ID : 1TLC
Title : THYMIDYLATE SYNTHASE COMPLEXED WITH DGMP AND FOLATE ANALOG 1843U89
Authors : Weichsel, A.; Montfort, W.R.; Ciesla, J.; Maley, F.
Deposited on : 1995-03-07
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

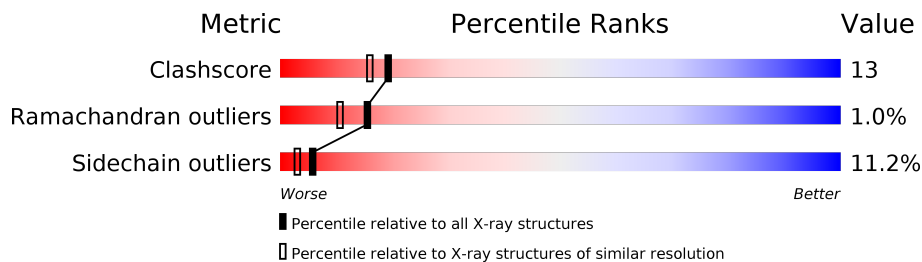
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 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	265	
1	B	265	

2 Entry composition [i](#)

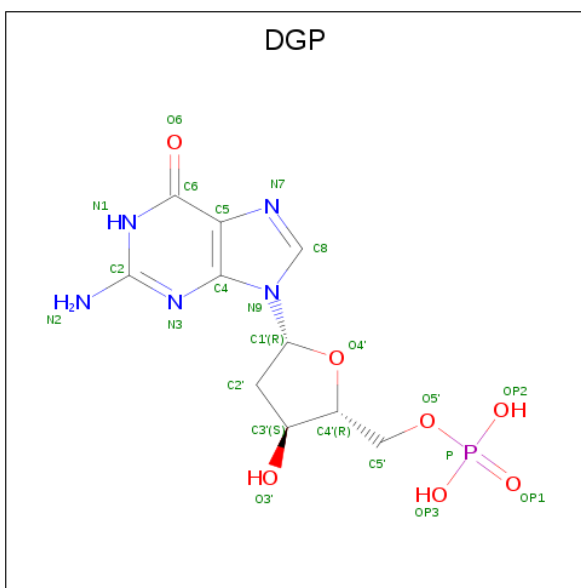
There are 4 unique types of molecules in this entry. The entry contains 4592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	Total 2153	C 1375	N 371	O 395	S 12	0	0	0
1	B	265	Total 2153	C 1375	N 371	O 395	S 12	0	0	0

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (three-letter code: DGP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	B	1	Total 23	C 10	N 5	O 7	P 1	0	0

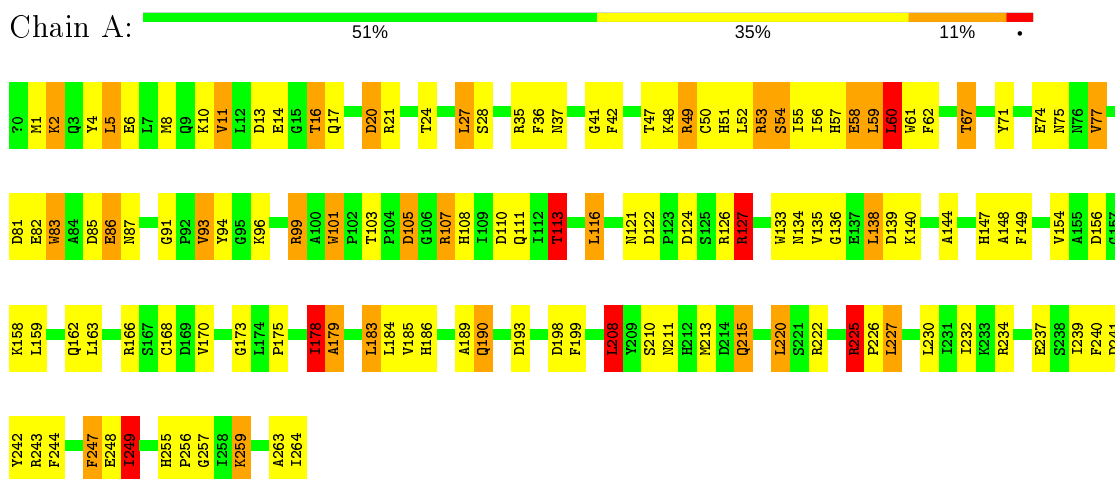
- Molecule 3 is S)-2-(5(((1,2-DIHYDRO-3-METHYL-1-OXOBENZO(F)QUINAZOLIN-9-YL)METHYL)AMINO)1-OXO-2-ISOINDOLINYL)GLUTARIC ACID (three-letter code: F89) (formula: C₂₇H₂₄N₄O₆).

3 Residue-property plots [i](#)

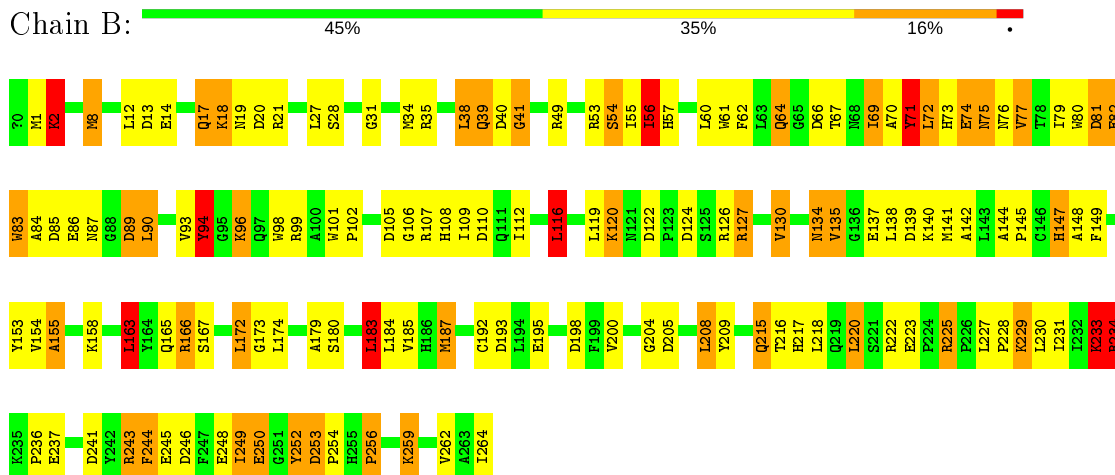
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: THYMIDYLATE SYNTHASE



- Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	127.14Å 127.14Å 67.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4592	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, F89, DGP

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	1.17	5/2210 (0.2%)	2.47	118/3000 (3.9%)
1	B	1.12	2/2210 (0.1%)	2.79	167/3000 (5.6%)
All	All	1.15	7/4420 (0.2%)	2.63	285/6000 (4.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CD-OE2	-6.21	1.18	1.25
1	A	105	ASP	C-N	-5.98	1.22	1.33
1	B	107	ARG	CZ-NH1	5.95	1.40	1.33
1	A	28	SER	CB-OG	-5.79	1.34	1.42
1	A	14	GLU	CD-OE1	5.46	1.31	1.25
1	A	168	CYS	CB-SG	-5.13	1.73	1.81
1	B	28	SER	CB-OG	-5.01	1.35	1.42

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH1	35.34	137.97	120.30
1	A	35	ARG	NE-CZ-NH1	30.58	135.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ARG	NE-CZ-NH2	-25.39	107.60	120.30
1	B	99	ARG	NE-CZ-NH2	23.38	131.99	120.30
1	B	49	ARG	NE-CZ-NH2	-20.23	110.19	120.30
1	B	243	ARG	NE-CZ-NH2	-18.80	110.90	120.30
1	B	198	ASP	CB-CG-OD1	16.62	133.26	118.30
1	B	139	ASP	CB-CG-OD1	16.01	132.71	118.30
1	B	234	ARG	NE-CZ-NH1	-15.55	112.52	120.30
1	B	246	ASP	CB-CG-OD2	15.54	132.28	118.30
1	A	4	TYR	CB-CG-CD2	15.07	130.04	121.00
1	B	127	ARG	NE-CZ-NH2	-14.71	112.94	120.30
1	B	53	ARG	NE-CZ-NH2	-14.69	112.95	120.30
1	B	99	ARG	NH1-CZ-NH2	-14.47	103.48	119.40
1	B	253	ASP	CB-CG-OD2	-14.14	105.57	118.30
1	A	4	TYR	CB-CG-CD1	-13.77	112.74	121.00
1	A	198	ASP	CB-CG-OD1	13.65	130.59	118.30
1	B	222	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	A	126	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	B	243	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	A	193	ASP	CB-CG-OD2	-12.26	107.26	118.30
1	B	205	ASP	CB-CG-OD2	11.98	129.08	118.30
1	B	107	ARG	NE-CZ-NH1	11.67	126.13	120.30
1	B	107	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	B	56	ILE	CA-CB-CG2	11.55	134.00	110.90
1	B	122	ASP	CB-CG-OD1	11.33	128.49	118.30
1	A	127	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	B	21	ARG	CD-NE-CZ	11.23	139.32	123.60
1	B	71	TYR	CB-CG-CD1	11.23	127.74	121.00
1	B	14	GLU	OE1-CD-OE2	11.19	136.72	123.30
1	A	122	ASP	CB-CG-OD1	-11.04	108.36	118.30
1	A	74	GLU	OE1-CD-OE2	-10.58	110.61	123.30
1	B	89	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	B	20	ASP	CB-CG-OD1	-10.49	108.86	118.30
1	B	155	ALA	N-CA-CB	10.46	124.74	110.10
1	B	35	ARG	CD-NE-CZ	10.37	138.12	123.60
1	B	35	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	222	ARG	NE-CZ-NH1	-10.19	115.20	120.30
1	B	166	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	A	81	ASP	CB-CG-OD1	10.14	127.42	118.30
1	B	85	ASP	CB-CG-OD1	-9.91	109.38	118.30
1	B	21	ARG	NE-CZ-NH2	9.74	125.17	120.30
1	B	28	SER	N-CA-CB	-9.67	96.00	110.50
1	A	126	ARG	NE-CZ-NH1	9.62	125.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NH1-CZ-NH2	-9.61	108.83	119.40
1	B	73	HIS	CA-CB-CG	9.60	129.93	113.60
1	A	243	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	A	81	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	A	59	LEU	CB-CG-CD2	9.38	126.95	111.00
1	B	147	HIS	CA-CB-CG	9.37	129.53	113.60
1	A	178	ILE	CA-CB-CG2	9.31	129.51	110.90
1	B	73	HIS	N-CA-CB	9.30	127.33	110.60
1	B	85	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	126	ARG	NE-CZ-NH2	9.19	124.89	120.30
1	A	99	ARG	NE-CZ-NH2	9.17	124.88	120.30
1	B	94	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	B	64	GLN	CG-CD-OE1	8.96	139.52	121.60
1	A	105	ASP	CB-CG-OD1	-8.92	110.28	118.30
1	B	21	ARG	CA-CB-CG	8.86	132.88	113.40
1	B	149	PHE	N-CA-CB	-8.72	94.90	110.60
1	A	103	THR	CA-CB-CG2	8.71	124.60	112.40
1	B	130	VAL	CA-CB-CG1	8.70	123.95	110.90
1	B	81	ASP	CB-CG-OD1	8.63	126.07	118.30
1	B	71	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	B	172	LEU	CB-CG-CD2	-8.59	96.40	111.00
1	B	14	GLU	CG-CD-OE2	-8.55	101.20	118.30
1	B	53	ARG	NH1-CZ-NH2	8.46	128.71	119.40
1	B	99	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	B	86	GLU	OE1-CD-OE2	-8.42	113.19	123.30
1	B	172	LEU	CA-CB-CG	8.34	134.49	115.30
1	B	187	MET	CG-SD-CE	-8.33	86.87	100.20
1	A	1	MET	CG-SD-CE	8.32	113.52	100.20
1	B	72	LEU	CA-CB-CG	8.30	134.40	115.30
1	A	220	LEU	CA-CB-CG	8.16	134.07	115.30
1	B	237	GLU	CG-CD-OE2	8.11	134.52	118.30
1	B	107	ARG	CG-CD-NE	8.00	128.60	111.80
1	A	116	LEU	CB-CG-CD1	-7.98	97.43	111.00
1	A	237	GLU	CA-CB-CG	7.92	130.82	113.40
1	B	250	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	A	51	HIS	CA-CB-CG	-7.89	100.18	113.60
1	B	124	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	A	13	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	48	LYS	N-CA-CB	7.82	124.67	110.60
1	B	40	ASP	CB-CG-OD2	7.82	125.33	118.30
1	B	163	LEU	CB-CG-CD2	7.73	124.15	111.00
1	B	234	ARG	NH1-CZ-NH2	7.67	127.83	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	TYR	CB-CG-CD1	-7.65	116.41	121.00
1	B	64	GLN	CG-CD-NE2	-7.59	98.48	116.70
1	B	126	ARG	NH1-CZ-NH2	-7.55	111.09	119.40
1	B	140	LYS	CB-CG-CD	7.50	131.09	111.60
1	B	237	GLU	CB-CG-CD	7.42	134.25	114.20
1	B	126	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	11	VAL	CA-CB-CG1	7.40	122.00	110.90
1	B	99	ARG	N-CA-CB	-7.40	97.28	110.60
1	B	49	ARG	NH1-CZ-NH2	7.36	127.49	119.40
1	B	61	TRP	O-C-N	-7.33	110.97	122.70
1	A	71	TYR	CB-CG-CD2	7.33	125.40	121.00
1	A	225	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	A	74	GLU	CG-CD-OE1	7.33	132.95	118.30
1	B	225	ARG	CG-CD-NE	-7.32	96.43	111.80
1	A	139	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	230	LEU	CB-CG-CD2	-7.16	98.82	111.00
1	B	38	LEU	CA-CB-CG	7.15	131.75	115.30
1	B	56	ILE	CB-CA-C	7.14	125.87	111.60
1	B	184	LEU	CB-CG-CD2	-7.12	98.89	111.00
1	A	107	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	49	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	248	GLU	OE1-CD-OE2	7.09	131.80	123.30
1	B	87	ASN	CA-CB-CG	7.06	128.93	113.40
1	A	113	THR	CA-CB-CG2	7.04	122.25	112.40
1	A	127	ARG	NH1-CZ-NH2	-7.03	111.66	119.40
1	A	20	ASP	CB-CA-C	7.03	124.45	110.40
1	B	107	ARG	CA-CB-CG	7.01	128.83	113.40
1	A	77	VAL	CA-CB-CG2	-6.96	100.47	110.90
1	B	66	ASP	CA-C-N	-6.95	101.92	117.20
1	A	138	LEU	CA-CB-CG	6.91	131.20	115.30
1	B	77	VAL	N-CA-CB	6.91	126.70	111.50
1	B	86	GLU	CA-CB-CG	6.91	128.59	113.40
1	B	198	ASP	OD1-CG-OD2	-6.90	110.19	123.30
1	B	252	TYR	CB-CG-CD2	6.88	125.13	121.00
1	A	208	LEU	CB-CG-CD1	6.86	122.67	111.00
1	A	71	TYR	CB-CG-CD1	-6.86	116.89	121.00
1	B	2	LYS	CB-CG-CD	6.84	129.37	111.60
1	B	250	GLU	CG-CD-OE2	-6.81	104.67	118.30
1	A	20	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	A	83	TRP	CB-CA-C	6.80	124.00	110.40
1	B	243	ARG	O-C-N	6.80	133.57	122.70
1	A	247	PHE	CB-CG-CD2	-6.77	116.06	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	MET	CB-CA-C	6.76	123.92	110.40
1	A	74	GLU	CB-CG-CD	6.74	132.40	114.20
1	A	198	ASP	OD1-CG-OD2	-6.72	110.53	123.30
1	A	85	ASP	CB-CA-C	6.64	123.69	110.40
1	B	86	GLU	CG-CD-OE1	6.64	131.57	118.30
1	A	225	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	27	LEU	CA-CB-CG	6.60	130.48	115.30
1	B	243	ARG	N-CA-CB	6.59	122.46	110.60
1	A	225	ARG	NH1-CZ-NH2	-6.53	112.21	119.40
1	B	108	HIS	N-CA-CB	6.52	122.34	110.60
1	B	234	ARG	CD-NE-CZ	6.50	132.71	123.60
1	A	178	ILE	CB-CA-C	6.47	124.54	111.60
1	B	75	ASN	OD1-CG-ND2	-6.46	107.03	121.90
1	A	87	ASN	CB-CG-OD1	-6.44	108.72	121.60
1	A	101	TRP	N-CA-CB	-6.43	99.02	110.60
1	B	105	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	A	60	LEU	CB-CA-C	6.42	122.39	110.20
1	B	225	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	20	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	17	GLN	CA-CB-CG	6.38	127.44	113.40
1	A	166	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	B	1	MET	CB-CA-C	6.34	123.08	110.40
1	B	140	LYS	CA-CB-CG	6.29	127.25	113.40
1	B	137	GLU	CG-CD-OE1	-6.25	105.80	118.30
1	B	60	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	A	96	LYS	N-CA-CB	-6.20	99.44	110.60
1	B	135	VAL	C-N-CA	6.17	135.26	122.30
1	B	208	LEU	CA-CB-CG	6.17	129.48	115.30
1	B	140	LYS	CG-CD-CE	6.13	130.28	111.90
1	B	110	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	244	PHE	N-CA-CB	-6.09	99.64	110.60
1	A	237	GLU	CB-CG-CD	6.08	130.62	114.20
1	A	6	GLU	N-CA-CB	6.08	121.54	110.60
1	A	99	ARG	NH1-CZ-NH2	-6.08	112.72	119.40
1	B	153	TYR	N-CA-CB	-6.07	99.67	110.60
1	A	190	GLN	CG-CD-OE1	-6.06	109.48	121.60
1	A	50	CYS	CA-CB-SG	-6.06	103.09	114.00
1	A	111	GLN	CG-CD-NE2	5.99	131.08	116.70
1	B	148	ALA	N-CA-CB	-5.98	101.73	110.10
1	A	148	ALA	N-CA-CB	-5.98	101.73	110.10
1	A	57	HIS	CA-CB-CG	-5.97	103.45	113.60
1	B	64	GLN	N-CA-CB	5.97	121.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ASP	CA-CB-CG	5.96	126.50	113.40
1	A	227	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	B	163	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	225	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	B	195	GLU	CG-CD-OE2	5.92	130.13	118.30
1	B	86	GLU	CB-CG-CD	5.91	130.16	114.20
1	B	249	ILE	CA-CB-CG2	5.84	122.58	110.90
1	B	90	LEU	N-CA-CB	-5.83	98.74	110.40
1	A	60	LEU	C-N-CA	5.83	136.26	121.70
1	B	139	ASP	OD1-CG-OD2	-5.82	112.24	123.30
1	A	213	MET	N-CA-CB	5.82	121.07	110.60
1	A	11	VAL	CB-CA-C	5.80	122.42	111.40
1	A	198	ASP	CB-CA-C	-5.79	98.83	110.40
1	B	237	GLU	OE1-CD-OE2	-5.77	116.37	123.30
1	B	56	ILE	CA-C-N	5.77	129.89	117.20
1	B	253	ASP	CB-CA-C	5.75	121.89	110.40
1	A	2	LYS	CD-CE-NZ	5.74	124.89	111.70
1	A	14	GLU	CG-CD-OE1	-5.72	106.86	118.30
1	A	41	GLY	O-C-N	5.72	131.85	122.70
1	A	67	THR	CA-CB-OG1	-5.71	97.00	109.00
1	A	140	LYS	C-N-CA	5.71	135.98	121.70
1	B	27	LEU	N-CA-CB	5.71	121.82	110.40
1	B	39	GLN	CA-CB-CG	5.71	125.96	113.40
1	B	223	GLU	O-C-N	5.71	131.95	121.10
1	A	199	PHE	CB-CG-CD2	-5.69	116.82	120.80
1	A	257	GLY	CA-C-O	5.67	130.81	120.60
1	B	183	LEU	CB-CA-C	5.66	120.94	110.20
1	B	253	ASP	OD1-CG-OD2	5.65	134.04	123.30
1	A	222	ARG	CG-CD-NE	-5.64	99.94	111.80
1	A	159	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	B	230	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	72	LEU	CB-CA-C	5.63	120.90	110.20
1	B	130	VAL	N-CA-CB	5.62	123.86	111.50
1	B	223	GLU	CG-CD-OE2	5.62	129.53	118.30
1	A	54	SER	CB-CA-C	5.61	120.77	110.10
1	B	244	PHE	CB-CA-C	5.61	121.61	110.40
1	B	195	GLU	CG-CD-OE1	-5.60	107.10	118.30
1	A	156	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	183	LEU	CB-CG-CD2	-5.57	101.52	111.00
1	A	1	MET	CB-CA-C	-5.57	99.26	110.40
1	A	189	ALA	O-C-N	-5.55	113.81	122.70
1	B	64	GLN	CB-CG-CD	5.54	126.00	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	PHE	CB-CG-CD1	5.53	124.67	120.80
1	B	180	SER	CA-CB-OG	5.53	126.14	111.20
1	B	223	GLU	N-CA-CB	5.53	120.56	110.60
1	B	70	ALA	CB-CA-C	5.53	118.39	110.10
1	A	173	GLY	N-CA-C	5.52	126.90	113.10
1	B	105	ASP	N-CA-C	5.51	125.88	111.00
1	B	116	LEU	CA-C-O	5.51	131.67	120.10
1	B	8	MET	CG-SD-CE	-5.50	91.39	100.20
1	A	49	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	A	211	ASN	CB-CG-OD1	5.50	132.60	121.60
1	A	158	LYS	O-C-N	5.47	131.45	122.70
1	B	233	LYS	CA-CB-CG	5.47	125.43	113.40
1	B	246	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	B	185	VAL	CA-CB-CG1	5.46	119.08	110.90
1	B	107	ARG	CB-CG-CD	5.45	125.78	111.60
1	A	140	LYS	CD-CE-NZ	5.45	124.24	111.70
1	A	52	LEU	CB-CA-C	5.44	120.54	110.20
1	A	21	ARG	N-CA-CB	-5.43	100.82	110.60
1	B	138	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	A	16	THR	CA-CB-CG2	5.43	120.00	112.40
1	B	13	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	217	HIS	O-C-N	-5.42	114.03	122.70
1	A	234	ARG	N-CA-CB	-5.41	100.86	110.60
1	B	72	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	A	185	VAL	O-C-N	-5.39	114.08	122.70
1	A	149	PHE	N-CA-CB	-5.36	100.95	110.60
1	B	27	LEU	N-CA-C	-5.36	96.53	111.00
1	B	18	LYS	CA-CB-CG	5.34	125.15	113.40
1	A	28	SER	N-CA-CB	-5.33	102.50	110.50
1	B	98	TRP	CA-CB-CG	5.31	123.79	113.70
1	B	106	GLY	N-CA-C	5.31	126.38	113.10
1	B	192	CYS	CA-CB-SG	-5.31	104.45	114.00
1	A	24	THR	N-CA-CB	5.31	120.38	110.30
1	A	121	ASN	N-CA-C	5.29	125.29	111.00
1	B	256	PRO	O-C-N	5.27	132.16	123.20
1	B	137	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	B	81	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	193	ASP	OD1-CG-OD2	5.24	133.26	123.30
1	B	135	VAL	O-C-N	-5.23	114.31	123.20
1	B	84	ALA	N-CA-CB	-5.22	102.79	110.10
1	A	10	LYS	CB-CA-C	5.22	120.84	110.40
1	B	62	PHE	CB-CG-CD2	-5.21	117.15	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	LEU	CB-CA-C	5.21	120.10	110.20
1	B	173	GLY	CA-C-O	-5.20	111.24	120.60
1	B	209	TYR	CB-CG-CD2	5.20	124.12	121.00
1	B	105	ASP	C-N-CA	5.20	133.21	122.30
1	A	75	ASN	CB-CG-OD1	-5.18	111.24	121.60
1	A	249	ILE	CA-CB-CG2	5.18	121.25	110.90
1	A	17	GLN	OE1-CD-NE2	5.17	133.79	121.90
1	B	76	ASN	CB-CA-C	5.17	120.73	110.40
1	A	178	ILE	C-N-CA	5.15	134.57	121.70
1	B	193	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	19	ASN	N-CA-C	-5.12	97.17	111.00
1	A	259	LYS	N-CA-CB	5.10	119.78	110.60
1	A	259	LYS	O-C-N	5.10	130.86	122.70
1	A	82	GLU	CG-CD-OE1	5.09	128.49	118.30
1	A	179	ALA	N-CA-CB	5.09	117.23	110.10
1	B	108	HIS	CA-CB-CG	-5.09	104.95	113.60
1	B	122	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	241	ASP	CA-C-O	-5.07	109.46	120.10
1	B	41	GLY	O-C-N	5.06	130.79	122.70
1	B	124	ASP	OD1-CG-OD2	5.06	132.91	123.30
1	B	246	ASP	CA-CB-CG	5.04	124.48	113.40
1	B	200	VAL	CA-CB-CG1	-5.03	103.35	110.90
1	A	144	ALA	N-CA-CB	-5.03	103.06	110.10
1	A	86	GLU	CA-CB-CG	5.03	124.46	113.40
1	A	4	TYR	N-CA-CB	-5.01	101.58	110.60
1	A	93	VAL	CA-CB-CG1	-5.01	103.39	110.90
1	B	90	LEU	CA-C-O	5.01	130.62	120.10
1	A	5	LEU	CB-CA-C	5.01	119.71	110.20
1	A	162	GLN	CG-CD-NE2	5.01	128.72	116.70
1	A	148	ALA	N-CA-C	5.00	124.50	111.00
1	B	82	GLU	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	HIS	Mainchain
1	A	127	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	127	ARG	Sidechain

5.2 Too-close contacts [\(i\)](#)

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	2153	0	2079	52	0
1	B	2153	0	2080	66	0
2	A	23	0	12	0	0
2	B	23	0	12	2	0
3	A	37	0	23	2	0
3	B	37	0	22	5	0
4	A	107	0	0	1	0
4	B	59	0	0	2	0
All	All	4592	0	4228	112	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 13.

All (112) 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)
3:B:266:F89:C	3:B:266:F89:HG1	1.89	1.02
1:B:183:LEU:HD22	1:B:187:MET:HE2	1.46	0.97
1:A:215:GLN:HE21	1:A:215:GLN:H	1.18	0.91
1:B:259:LYS:HB3	4:B:400:HOH:O	1.78	0.82
1:A:53:ARG:HH11	1:A:53:ARG:HG3	1.50	0.76
1:B:259:LYS:HD2	1:B:259:LYS:H	1.56	0.70
1:B:57:HIS:HD2	1:B:71:TYR:OH	1.75	0.70
1:A:16:THR:HG21	1:B:155:ALA:HB1	1.73	0.70
1:B:56:ILE:C	1:B:56:ILE:HD13	2.13	0.69
1:B:55:ILE:HD13	1:B:179:ALA:HB3	1.74	0.69
1:B:69:ILE:HG22	1:B:72:LEU:HD12	1.76	0.68
1:A:36:PHE:CZ	1:A:178:ILE:HD13	2.30	0.67
1:A:215:GLN:NE2	1:A:215:GLN:H	1.88	0.67
1:B:69:ILE:HG21	1:B:80:TRP:HB3	1.76	0.67
1:B:233:LYS:HD3	1:B:245:GLU:O	1.96	0.66
1:B:234:ARG:O	1:B:236:PRO:HD3	1.96	0.64
1:B:69:ILE:HG23	1:B:90:LEU:HD11	1.81	0.62
1:B:41:GLY:HA2	1:B:229:LYS:HE3	1.82	0.61
1:B:183:LEU:HD22	1:B:187:MET:CE	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HD12	1:B:244:PHE:HD1	1.65	0.61
1:B:82:GLU:HG2	1:B:264:ILE:HG21	1.82	0.59
1:B:39:GLN:HE21	1:B:158:LYS:HE3	1.67	0.59
1:B:54:SER:HB2	3:B:266:F89:H17	1.84	0.58
1:A:136:GLY:HA2	1:B:109:ILE:HD11	1.86	0.58
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.87	0.57
1:A:53:ARG:HG3	1:A:53:ARG:NH1	2.20	0.57
1:A:135:VAL:HG12	1:B:109:ILE:HD13	1.87	0.56
1:B:83:TRP:CZ3	3:B:266:F89:H5	2.40	0.56
1:A:53:ARG:HA	1:A:244:PHE:HE1	1.70	0.56
1:B:12:LEU:HD11	1:B:216:THR:CG2	2.35	0.56
1:A:8:MET:HE3	1:A:220:LEU:HD13	1.88	0.55
1:A:55:ILE:HD13	1:A:179:ALA:HB3	1.87	0.55
1:A:16:THR:HG22	4:B:424:HOH:O	2.07	0.55
1:A:215:GLN:N	1:A:215:GLN:HE21	1.99	0.54
1:B:252:TYR:CE2	1:B:254:PRO:HG3	2.42	0.54
1:A:110:ASP:OD2	1:A:113:THR:HG23	2.08	0.53
1:B:69:ILE:CG2	1:B:90:LEU:HD11	2.38	0.53
1:B:116:LEU:HD13	1:B:120:LYS:HD2	1.91	0.53
1:A:56:ILE:HG22	1:A:60:LEU:HD22	1.91	0.53
1:B:69:ILE:HG12	1:B:81:ASP:OD1	2.09	0.53
1:B:74:GLU:HG2	1:B:75:ASN:OD1	2.09	0.51
1:A:133:TRP:CZ2	1:A:138:LEU:HD21	2.45	0.51
1:B:55:ILE:HD13	1:B:179:ALA:CB	2.38	0.51
1:B:231:ILE:HD13	1:B:250:GLU:HG3	1.93	0.51
1:A:83:TRP:CH2	3:A:266:F89:H5	2.44	0.51
1:B:165:GLN:O	1:B:204:GLY:N	2.37	0.51
1:A:67:THR:HB	1:A:91:GLY:O	2.11	0.50
1:B:93:VAL:O	1:B:94:TYR:C	2.50	0.50
1:A:101:TRP:CE2	1:B:135:VAL:HB	2.47	0.49
1:B:12:LEU:HD11	1:B:216:THR:HG21	1.92	0.49
1:B:215:GLN:H	1:B:215:GLN:HE21	1.59	0.49
1:B:39:GLN:NE2	1:B:158:LYS:HE3	2.27	0.49
1:A:8:MET:CE	1:A:220:LEU:HD13	2.43	0.48
1:A:5:LEU:HD11	1:A:47:THR:HG21	1.94	0.48
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.22	0.48
1:B:172:LEU:HD21	1:B:262:VAL:HG22	1.96	0.48
1:B:141:MET:SD	1:B:145:PRO:HD3	2.53	0.48
1:B:225:ARG:HD2	1:B:253:ASP:O	2.12	0.48
1:B:218:LEU:O	1:B:218:LEU:HD12	2.14	0.47
1:A:53:ARG:CG	1:A:53:ARG:NH1	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:HA2	1:B:109:ILE:CD1	2.44	0.47
1:B:183:LEU:HD13	1:B:187:MET:HE1	1.97	0.47
1:B:8:MET:HB3	1:B:220:LEU:HD11	1.97	0.47
1:B:96:LYS:NZ	1:B:102:PRO:HG3	2.30	0.47
1:A:36:PHE:CZ	1:A:178:ILE:CD1	2.98	0.46
1:A:55:ILE:HD13	1:A:179:ALA:CB	2.46	0.46
1:B:147:HIS:HB2	1:B:163:LEU:HD21	1.97	0.46
1:B:2:LYS:HD2	1:B:2:LYS:H	1.80	0.46
1:A:11:VAL:HG22	1:A:208:LEU:HD22	1.98	0.45
1:A:127:ARG:NH2	2:B:265:DGP:OP3	2.33	0.45
1:A:215:GLN:NE2	1:A:215:GLN:N	2.63	0.44
1:A:54:SER:HB2	1:A:77:VAL:HG22	1.98	0.44
1:A:16:THR:HG21	1:B:155:ALA:CB	2.46	0.44
1:A:42:PHE:CD2	1:A:249:ILE:HD11	2.52	0.44
1:A:113:THR:HG22	1:A:240:PHE:CE2	2.53	0.44
1:A:56:ILE:HG12	1:A:183:LEU:HD21	1.99	0.44
1:B:154:VAL:HA	1:B:158:LYS:O	2.17	0.44
1:A:190:GLN:NE2	1:A:242:TYR:OH	2.46	0.44
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.47	0.44
1:B:74:GLU:CG	1:B:74:GLU:O	2.66	0.44
1:B:90:LEU:O	1:B:142:ALA:N	2.51	0.44
1:B:228:PRO:HB2	1:B:249:ILE:HG13	1.99	0.44
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.80	0.43
1:A:154:VAL:O	1:B:18:LYS:HE2	2.18	0.43
1:A:36:PHE:CE1	1:A:178:ILE:CD1	3.01	0.43
1:A:184:LEU:HA	1:A:184:LEU:HD12	1.89	0.43
1:A:58:GLU:O	1:A:61:TRP:HB3	2.19	0.43
1:A:49:ARG:HD2	1:A:49:ARG:HH11	1.57	0.42
1:B:166:ARG:HG3	1:B:167:SER:N	2.33	0.42
1:B:12:LEU:HD11	1:B:216:THR:HG22	2.00	0.42
1:A:263:ALA:O	3:A:266:F89:H3M1	2.19	0.42
1:A:225:ARG:HB3	1:A:226:PRO:HD2	2.02	0.42
1:A:255:HIS:HB3	1:A:256:PRO:HD2	2.02	0.42
1:B:259:LYS:HD2	1:B:259:LYS:N	2.31	0.42
1:A:186:HIS:CE1	4:A:289:HOH:O	2.72	0.42
1:A:232:ILE:HG12	1:A:247:PHE:CD1	2.55	0.42
1:B:67:THR:HG21	1:B:96:LYS:HB2	2.01	0.42
1:B:69:ILE:CG2	1:B:80:TRP:HB3	2.45	0.42
1:B:183:LEU:HD13	1:B:187:MET:CE	2.50	0.42
1:A:11:VAL:HG22	1:A:208:LEU:CD2	2.50	0.41
1:A:147:HIS:HB2	1:A:163:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:TYR:CZ	1:B:254:PRO:HG3	2.55	0.41
1:B:174:LEU:HA	1:B:174:LEU:HD12	1.82	0.41
1:A:124:ASP:OD1	1:B:18:LYS:HD2	2.20	0.41
1:A:127:ARG:HH21	2:B:265:DGP:P	2.41	0.41
1:B:79:ILE:HG23	1:B:80:TRP:N	2.36	0.41
1:B:80:TRP:CE2	3:B:266:F89:H7	2.55	0.41
1:B:101:TRP:CH2	1:B:134:ASN:HA	2.56	0.41
1:B:112:ILE:O	1:B:116:LEU:HB2	2.21	0.40
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.94	0.40
1:B:144:ALA:HA	1:B:145:PRO:HD3	1.95	0.40
3:B:266:F89:H14	3:B:266:F89:C9	2.50	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	263/265 (99%)	256 (97%)	5 (2%)	2 (1%)	19	15
1	B	263/265 (99%)	250 (95%)	10 (4%)	3 (1%)	14	9
All	All	526/530 (99%)	506 (96%)	15 (3%)	5 (1%)	15	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	TYR
1	B	74	GLU
1	A	94	TYR
1	A	93	VAL
1	B	31	GLY

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	233/233 (100%)	210 (90%)	23 (10%)	8	5
1	B	233/233 (100%)	204 (88%)	29 (12%)	4	2
All	All	466/466 (100%)	414 (89%)	52 (11%)	6	3

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	20	ASP
1	A	27	LEU
1	A	37	ASN
1	A	53	ARG
1	A	59	LEU
1	A	60	LEU
1	A	86	GLU
1	A	105	ASP
1	A	107	ARG
1	A	113	THR
1	A	134	ASN
1	A	175	PRO
1	A	178	ILE
1	A	208	LEU
1	A	210	SER
1	A	215	GLN
1	A	227	LEU
1	A	239	ILE
1	A	241	ASP
1	A	249	ILE
1	A	259	LYS
1	A	264	ILE
1	B	2	LYS
1	B	17	GLN
1	B	38	LEU
1	B	54	SER

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Mol	Chain	Res	Type
1	B	56	ILE
1	B	64	GLN
1	B	69	ILE
1	B	71	TYR
1	B	77	VAL
1	B	83	TRP
1	B	89	ASP
1	B	96	LYS
1	B	116	LEU
1	B	120	LYS
1	B	130	VAL
1	B	134	ASN
1	B	163	LEU
1	B	183	LEU
1	B	208	LEU
1	B	215	GLN
1	B	220	LEU
1	B	227	LEU
1	B	229	LYS
1	B	233	LYS
1	B	234	ARG
1	B	243	ARG
1	B	248	GLU
1	B	256	PRO
1	B	259	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	37	ASN
1	A	73	HIS
1	A	97	GLN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	190	GLN
1	A	215	GLN
1	B	57	HIS
1	B	117	ASN
1	B	118	GLN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	151	GLN
1	B	215	GLN
1	B	217	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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
2	DGP	B	265	-	22,25,25	1.53	7 (31%)	26,38,38	2.15	7 (26%)
3	F89	A	266	-	34,41,41	2.17	6 (17%)	45,60,60	5.20	18 (40%)
2	DGP	A	265	-	22,25,25	1.92	6 (27%)	26,38,38	4.05	11 (42%)
3	F89	B	266	-	34,41,41	2.53	10 (29%)	45,60,60	5.59	17 (37%)

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
2	DGP	B	265	-	-	1/6/22/22	0/3/3/3
3	F89	A	266	-	-	6/12/30/30	0/5/5/5
2	DGP	A	265	-	-	2/6/22/22	0/3/3/3
3	F89	B	266	-	-	6/12/30/30	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	266	F89	C19-N	7.67	1.52	1.46
3	A	266	F89	C19-N	7.17	1.52	1.46
3	B	266	F89	C3-N2	6.62	1.45	1.34
3	A	266	F89	C3-N2	6.37	1.45	1.34
2	A	265	DGP	C5'-C4'	5.36	1.68	1.51
3	B	266	F89	CA-N	5.15	1.54	1.47
3	B	266	F89	C4A-N4	4.63	1.45	1.37
3	A	266	F89	C4A-N4	4.34	1.44	1.37
2	A	265	DGP	O5'-C5'	-4.13	1.28	1.44
3	A	266	F89	C-N	-3.60	1.32	1.36
3	B	266	F89	CB-CA	3.01	1.57	1.53
3	B	266	F89	C-N	-3.00	1.33	1.36
2	B	265	DGP	C2'-C1'	2.83	1.60	1.52
2	A	265	DGP	C1'-N9	-2.73	1.41	1.49
2	B	265	DGP	C2-N1	2.65	1.40	1.35
3	B	266	F89	C3-N4	-2.64	1.29	1.34
3	A	266	F89	C3-N4	-2.47	1.29	1.34
2	A	265	DGP	C2'-C3'	-2.43	1.46	1.52
2	B	265	DGP	C2-N2	-2.43	1.29	1.33
3	B	266	F89	C13-N12	2.35	1.45	1.38
2	B	265	DGP	P-OP1	-2.29	1.43	1.50
3	B	266	F89	CB-CG	2.18	1.62	1.52
2	A	265	DGP	C2-N2	-2.17	1.29	1.33
2	A	265	DGP	C2'-C1'	2.16	1.58	1.52
2	B	265	DGP	C5-C4	-2.16	1.35	1.40
2	B	265	DGP	P-OP2	-2.14	1.46	1.54
3	B	266	F89	C1-N2	2.08	1.36	1.33
3	A	266	F89	C10-C9	2.08	1.42	1.37
2	B	265	DGP	P-OP3	-2.00	1.47	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	F89	C19-N-CA	-17.19	107.61	123.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	266	F89	O-C-N	16.20	137.40	125.24
3	B	266	F89	C19-N-CA	-15.85	108.87	123.71
3	A	266	F89	C3-N4-C4A	14.66	126.48	116.54
3	B	266	F89	C15-C19-N	14.07	106.87	102.18
3	A	266	F89	CA-N-C	13.26	142.39	121.82
3	A	266	F89	O-C-N	12.96	134.97	125.24
3	B	266	F89	CA-N-C	12.61	141.38	121.82
3	B	266	F89	C3-N4-C4A	11.81	124.55	116.54
2	A	265	DGP	C6-N1-C2	9.78	131.47	115.93
3	B	266	F89	C19-C15-C16	-9.34	103.92	109.75
2	A	265	DGP	C5-C6-N1	-9.01	111.11	123.43
2	A	265	DGP	P-O5'-C5'	8.61	142.01	118.30
3	B	266	F89	C19-N-C	-8.25	109.73	113.12
3	A	266	F89	C19-N-C	-7.59	110.00	113.12
3	A	266	F89	C1A-C1-N2	-7.48	117.45	124.09
3	B	266	F89	CB-CA-N	-7.32	104.28	112.65
3	A	266	F89	O-C-C16	-6.78	115.50	128.68
3	B	266	F89	O-C-C16	-6.56	115.93	128.68
3	B	266	F89	C1A-C1-N2	-6.55	118.28	124.09
2	B	265	DGP	C5-C6-N1	-6.33	114.77	123.43
2	A	265	DGP	N3-C2-N1	-6.28	118.84	127.22
3	B	266	F89	C15-C16-C	6.15	112.23	108.94
2	A	265	DGP	N2-C2-N1	5.98	126.55	117.25
3	A	266	F89	C15-C19-N	5.86	104.13	102.18
2	A	265	DGP	O5'-P-OP1	5.45	121.77	106.47
3	A	266	F89	C16-C-N	5.23	109.53	106.44
3	A	266	F89	CB-CG-CD	-4.96	102.92	113.59
2	A	265	DGP	C6-C5-C4	-4.64	116.36	120.80
2	B	265	DGP	C2-N3-C4	-4.38	110.36	115.36
3	A	266	F89	N4-C3-N2	-4.27	117.87	125.72
3	A	266	F89	C11-N12-C13	3.46	131.04	122.15
2	B	265	DGP	C6-N1-C2	3.42	121.36	115.93
3	A	266	F89	C13-C14-C15	-3.31	116.39	120.94
3	A	266	F89	C3M-C3-N2	3.28	122.27	117.15
2	A	265	DGP	C3'-C2'-C1'	-3.19	94.55	102.54
3	A	266	F89	C14-C13-N12	-3.19	112.66	120.77
3	A	266	F89	C19-C15-C16	-3.13	107.79	109.75
2	B	265	DGP	P-O5'-C5'	3.08	126.79	118.30
3	B	266	F89	N4-C3-N2	-2.97	120.27	125.72
2	A	265	DGP	O4'-C4'-C5'	-2.91	99.78	109.37
3	B	266	F89	C3M-C3-N2	2.89	121.66	117.15
2	B	265	DGP	C3'-C2'-C1'	-2.80	95.52	102.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	266	F89	C13-C14-C15	-2.71	117.21	120.94
2	A	265	DGP	C4-C5-N7	2.62	112.13	109.40
3	A	266	F89	C9-C10-C1B	-2.47	118.96	122.65
2	B	265	DGP	O4'-C4'-C3'	-2.42	100.02	105.67
3	B	266	F89	C19-C15-C14	2.28	134.13	127.61
3	A	266	F89	C18-C13-N12	2.28	125.69	120.97
2	A	265	DGP	C2-N3-C4	-2.23	112.81	115.36
3	B	266	F89	C11-N12-C13	-2.18	116.55	122.15
3	B	266	F89	CB-CG-CD	-2.14	108.98	113.59
2	B	265	DGP	O3'-C3'-C2'	-2.00	103.73	110.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	266	F89	CT-CA-CB-CG
3	A	266	F89	CA-CB-CG-CD
3	B	266	F89	CT-CA-N-C19
3	B	266	F89	CB-CA-N-C
3	B	266	F89	N-CA-CB-CG
3	B	266	F89	CT-CA-CB-CG
3	B	266	F89	CA-CB-CG-CD
3	A	266	F89	CB-CA-N-C
3	A	266	F89	CB-CA-N-C19
3	B	266	F89	CB-CA-N-C19
2	B	265	DGP	O4'-C4'-C5'-O5'
2	A	265	DGP	O4'-C4'-C5'-O5'
2	A	265	DGP	C3'-C4'-C5'-O5'
3	A	266	F89	N-CA-CB-CG
3	A	266	F89	C9-C11-N12-C13

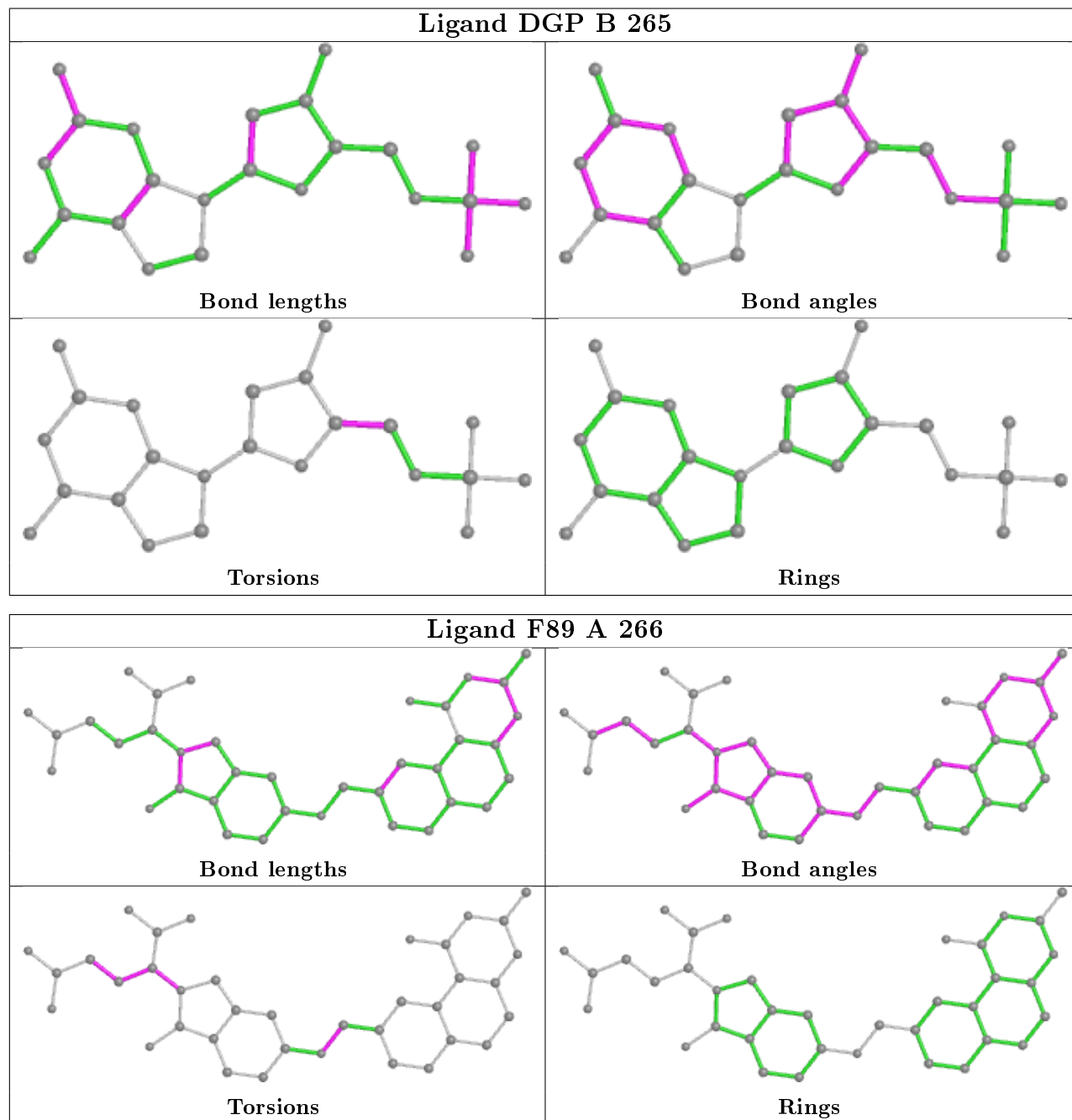
There are no ring outliers.

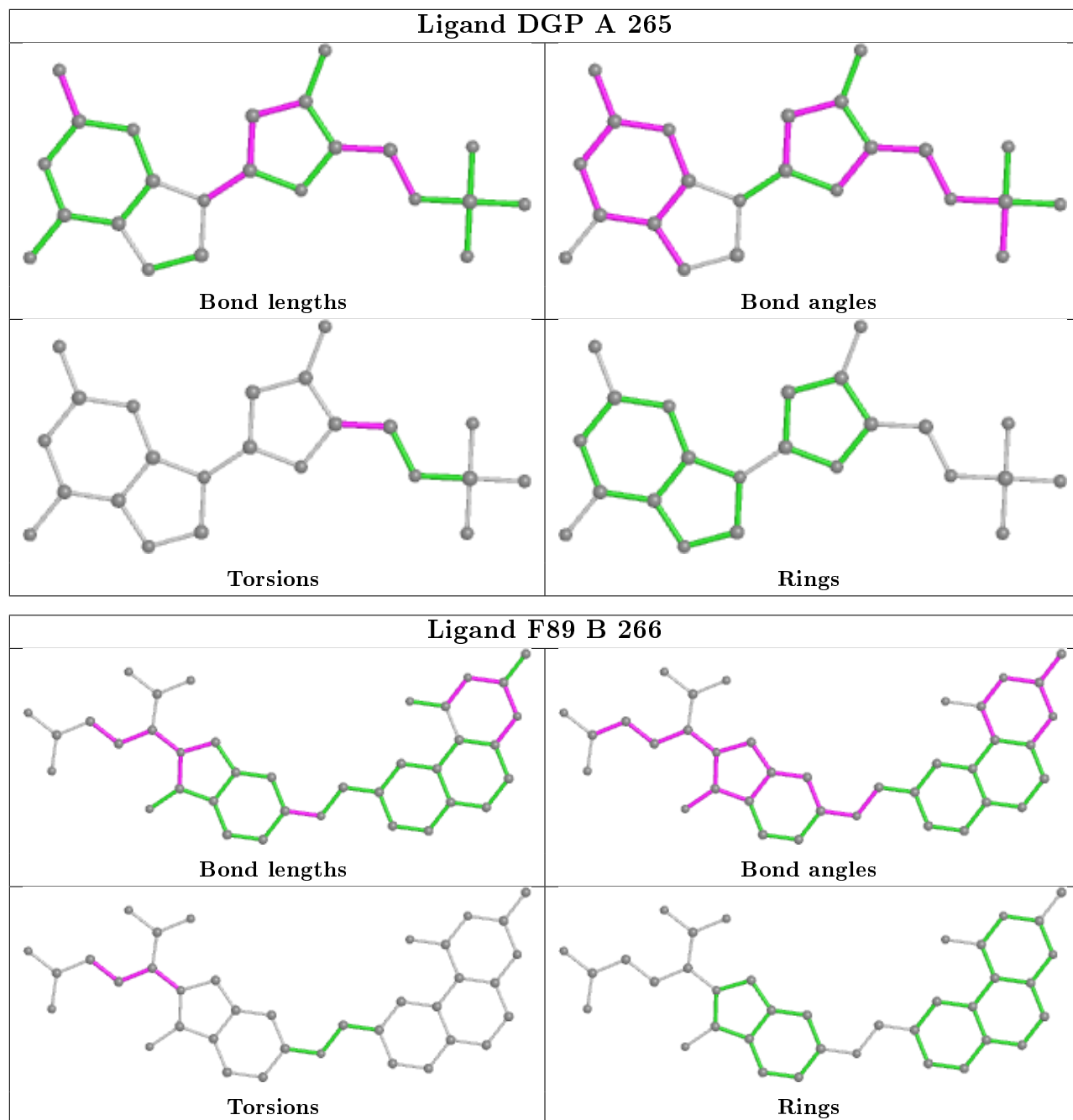
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	265	DGP	2	0
3	A	266	F89	2	0
3	B	266	F89	5	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 [\(i\)](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.