



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:13 PM UTC

PDB ID : 1TLC / pdb_00001tlc
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 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

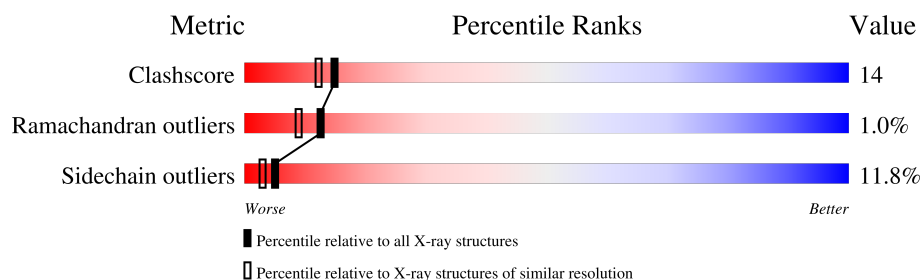
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 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	265	
1	B	265	

2 Entry composition [i](#)

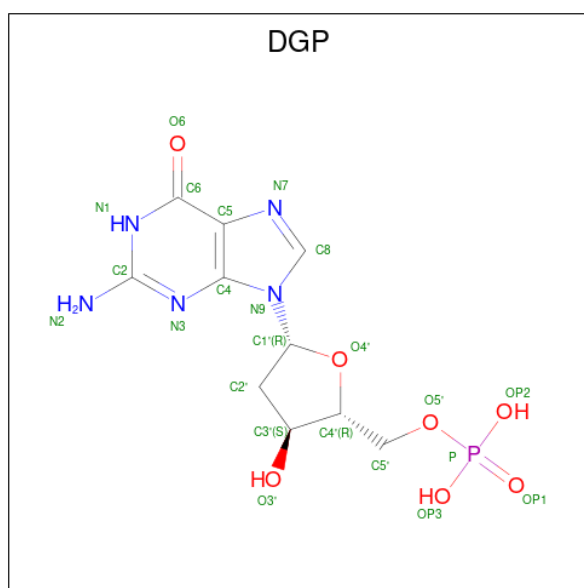
There are 4 unique types of molecules in this entry. The entry contains 4592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

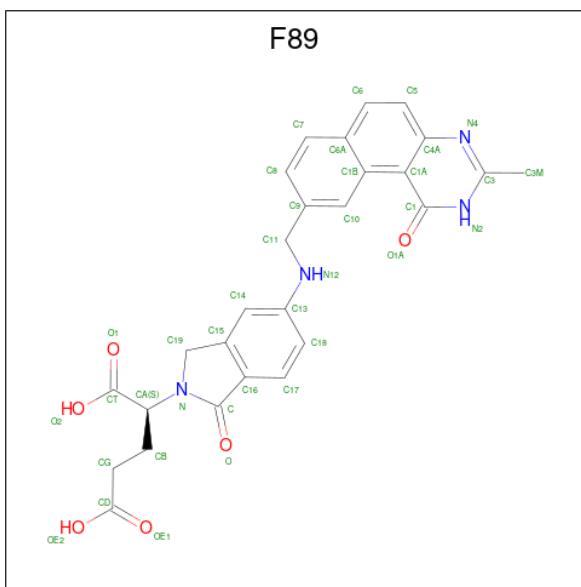
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			
1	B	265	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (CCD ID: DGP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- 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 (CCD ID: F89) (formula: $C_{27}H_{24}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 37	C 27	N 4	O 6	0	0
3	B	1	Total 37	C 27	N 4	O 6	0	0

- Molecule 4 is water.

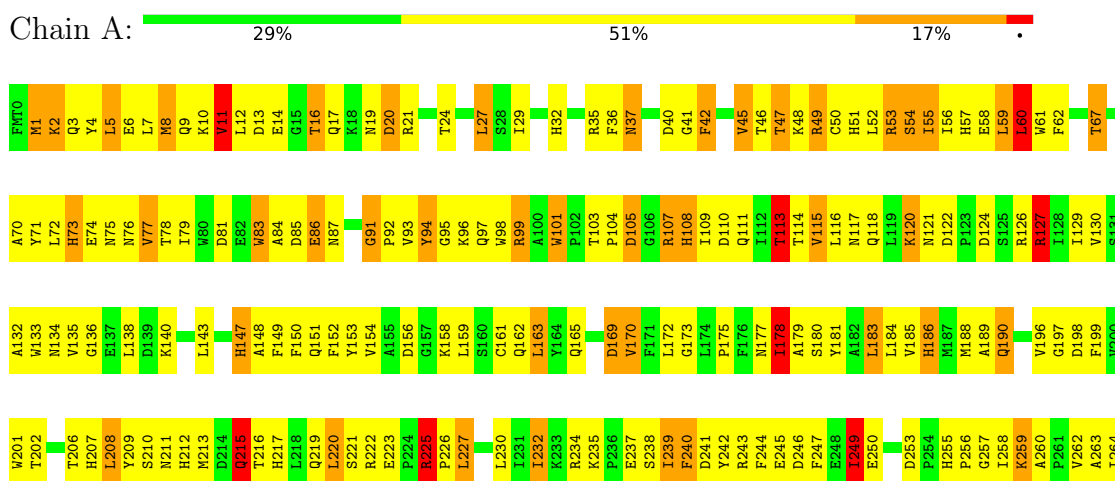
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	107	Total O 107 107	0	0
4	B	59	Total O 59 59	0	0

3 Residue-property plots

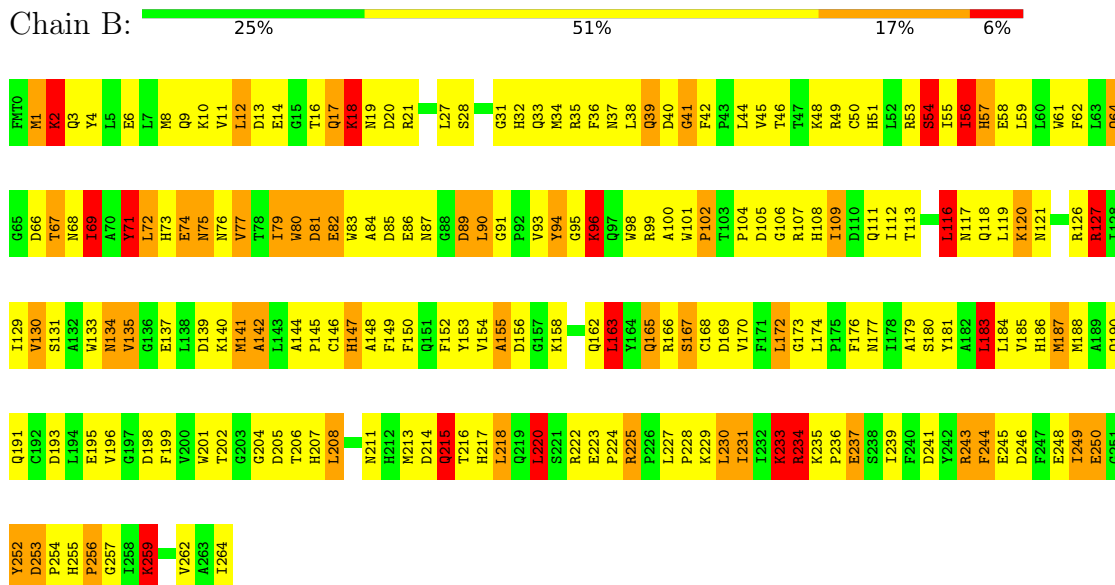
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Xtriage (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.	Xtriage
Total number of atoms	4592	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: DGP, FMT, F89

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	1.51	9/2210 (0.4%)	2.97	288/3000 (9.6%)
1	B	1.42	7/2210 (0.3%)	3.19	329/3000 (11.0%)
All	All	1.47	16/4420 (0.4%)	3.08	617/6000 (10.3%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ASP	C-N	-8.82	1.22	1.33
1	A	1	MET	C-N	-6.11	1.26	1.33
1	B	96	LYS	C-N	-5.90	1.25	1.33
1	B	176	PHE	C-N	-5.88	1.25	1.33
1	B	99	ARG	NE-CZ	5.87	1.39	1.33
1	B	107	ARG	CZ-NH1	5.74	1.40	1.32
1	A	108	HIS	C-N	-5.59	1.25	1.33
1	A	96	LYS	N-CA	5.57	1.53	1.46
1	B	102	PRO	C-O	5.51	1.29	1.23
1	A	32	HIS	CG-ND1	-5.45	1.32	1.38
1	B	207	HIS	CG-ND1	-5.35	1.32	1.38
1	A	54	SER	CA-C	5.29	1.60	1.52
1	A	156	ASP	C-O	5.29	1.30	1.23
1	B	27	LEU	CA-C	5.24	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ASN	N-CA	5.13	1.53	1.46
1	A	37	ASN	C-O	5.04	1.30	1.24

All (617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH1	16.47	137.97	121.50
1	B	87	ASN	CA-CB-CG	16.33	128.93	112.60
1	B	73	HIS	CA-CB-CG	16.13	129.93	113.80
1	B	147	HIS	CA-CB-CG	15.73	129.53	113.80
1	B	75	ASN	OD1-CG-ND2	-15.56	107.03	122.60
1	B	99	ARG	NE-CZ-NH2	14.21	131.99	119.20
1	A	35	ARG	NE-CZ-NH1	14.09	135.59	121.50
1	B	77	VAL	N-CA-CB	14.06	126.70	110.95
1	B	66	ASP	CA-CB-CG	13.90	126.50	112.60
1	B	56	ILE	CA-CB-CG2	13.82	134.00	110.50
1	A	51	HIS	CA-CB-CG	-13.62	100.18	113.80
1	A	35	ARG	NE-CZ-NH2	-12.89	107.60	119.20
1	B	237	GLU	CB-CG-CD	12.73	134.25	112.60
1	A	60	LEU	CA-C-N	12.17	136.26	120.44
1	A	60	LEU	C-N-CA	12.17	136.26	120.44
1	B	99	ARG	NH1-CZ-NH2	-12.17	103.48	119.30
1	A	37	ASN	OD1-CG-ND2	-12.07	110.53	122.60
1	B	73	HIS	N-CA-CB	11.97	127.33	109.98
1	B	64	GLN	CG-CD-NE2	-11.95	98.48	116.40
1	B	246	ASP	CA-CB-CG	11.88	124.48	112.60
1	A	74	GLU	CB-CG-CD	11.64	132.40	112.60
1	B	40	ASP	CA-CB-CG	11.55	124.15	112.60
1	B	223	GLU	O-C-N	11.52	131.95	121.35
1	A	17	GLN	OE1-CD-NE2	11.19	133.79	122.60
1	A	178	ILE	CA-CB-CG2	11.19	129.51	110.50
1	B	3	GLN	OE1-CD-NE2	-11.16	111.44	122.60
1	A	173	GLY	N-CA-C	11.04	126.90	112.77
1	B	235	LYS	CB-CA-C	10.89	120.24	110.44
1	B	56	ILE	CB-CA-C	10.86	125.87	111.97
1	B	61	TRP	O-C-N	-10.78	110.97	122.07
1	B	21	ARG	CD-NE-CZ	10.66	139.32	124.40
1	A	237	GLU	CB-CG-CD	10.60	130.62	112.60
1	A	215	GLN	OE1-CD-NE2	-10.46	112.14	122.60
1	A	211	ASN	CA-CB-CG	10.44	123.04	112.60
1	B	90	LEU	CA-C-O	10.44	130.62	119.14
1	A	122	ASP	CA-CB-CG	10.37	122.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	HIS	CA-CB-CG	-10.35	103.45	113.80
1	B	86	GLU	CB-CG-CD	10.33	130.16	112.60
1	B	10	LYS	CA-C-O	-10.32	109.61	120.55
1	A	140	LYS	CA-C-N	10.13	135.98	121.50
1	A	140	LYS	C-N-CA	10.13	135.98	121.50
1	B	68	ASN	OD1-CG-ND2	10.08	132.68	122.60
1	B	116	LEU	CA-C-O	10.07	131.67	120.90
1	A	178	ILE	CA-C-N	10.06	134.57	120.29
1	A	178	ILE	C-N-CA	10.06	134.57	120.29
1	A	150	PHE	CA-CB-CG	10.04	123.84	113.80
1	B	49	ARG	NE-CZ-NH2	-10.02	110.19	119.20
1	B	217	HIS	CA-C-N	9.90	133.55	120.28
1	B	217	HIS	C-N-CA	9.90	133.55	120.28
1	B	35	ARG	CD-NE-CZ	9.80	138.12	124.40
1	A	111	GLN	CG-CD-NE2	9.79	131.08	116.40
1	A	185	VAL	CA-C-N	9.77	133.37	120.28
1	A	185	VAL	C-N-CA	9.77	133.37	120.28
1	B	42	PHE	CA-C-O	-9.71	109.88	119.49
1	B	201	TRP	CA-C-O	-9.66	109.69	120.32
1	A	121	ASN	N-CA-C	9.59	125.29	113.50
1	A	178	ILE	CB-CA-C	9.56	124.54	112.02
1	B	21	ARG	CA-CB-CG	9.39	132.88	114.10
1	B	64	GLN	CG-CD-OE1	9.36	139.52	120.80
1	B	186	HIS	CA-C-N	9.34	133.14	120.44
1	B	186	HIS	C-N-CA	9.34	133.14	120.44
1	B	4	TYR	CA-C-N	9.24	132.67	120.28
1	B	4	TYR	C-N-CA	9.24	132.67	120.28
1	A	210	SER	CA-C-O	9.23	130.53	120.20
1	B	243	ARG	NE-CZ-NH2	-9.22	110.90	119.20
1	B	135	VAL	CA-C-O	9.18	130.60	121.05
1	B	214	ASP	CA-CB-CG	9.12	121.72	112.60
1	B	149	PHE	N-CA-CB	-9.07	94.90	111.13
1	B	243	ARG	O-C-N	9.06	133.57	123.25
1	B	99	ARG	N-CA-CB	-9.03	97.28	110.47
1	B	72	LEU	CA-C-O	-8.98	110.90	120.42
1	B	234	ARG	NE-CZ-NH1	-8.98	112.52	121.50
1	A	181	TYR	CA-C-O	-8.87	109.77	119.97
1	A	148	ALA	N-CA-C	8.86	124.50	112.90
1	B	108	HIS	CA-CB-CG	-8.85	104.95	113.80
1	A	57	HIS	CA-C-O	-8.82	111.20	120.55
1	A	62	PHE	CA-CB-CG	8.82	122.62	113.80
1	B	32	HIS	CA-C-O	-8.66	111.29	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	LYS	CB-CG-CD	8.61	131.09	111.30
1	A	97	GLN	OE1-CD-NE2	-8.58	114.02	122.60
1	B	155	ALA	N-CA-CB	8.57	124.74	110.77
1	A	149	PHE	CA-C-O	-8.53	109.73	120.14
1	B	79	ILE	O-C-N	8.53	130.25	121.89
1	B	130	VAL	N-CA-CB	8.45	123.86	111.52
1	B	135	VAL	CA-C-N	8.44	135.26	120.74
1	B	135	VAL	C-N-CA	8.44	135.26	120.74
1	A	67	THR	CA-CB-OG1	-8.40	97.00	109.60
1	A	237	GLU	CA-CB-CG	8.36	130.82	114.10
1	B	181	TYR	CA-C-O	-8.36	111.56	120.42
1	B	28	SER	N-CA-CB	-8.35	96.00	111.53
1	A	76	ASN	OD1-CG-ND2	8.33	130.93	122.60
1	B	75	ASN	CA-C-O	8.31	129.42	119.78
1	A	103	THR	CA-CB-CG2	8.29	124.60	110.50
1	B	51	HIS	CA-CB-CG	-8.27	105.53	113.80
1	B	140	LYS	CG-CD-CE	8.25	130.28	111.30
1	A	40	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	241	ASP	CA-C-O	-8.24	109.46	119.43
1	A	121	ASN	CA-CB-CG	-8.23	104.36	112.60
1	A	162	GLN	CG-CD-NE2	8.21	128.72	116.40
1	B	85	ASP	CA-CB-CG	8.19	120.79	112.60
1	B	106	GLY	N-CA-C	8.17	126.38	115.59
1	A	213	MET	CA-C-O	-8.12	112.29	120.82
1	B	66	ASP	CA-C-O	8.12	129.81	120.80
1	B	196	VAL	CA-C-O	-8.10	111.47	121.11
1	B	56	ILE	CA-C-O	-8.08	112.60	121.17
1	B	61	TRP	CA-C-N	8.07	130.93	120.44
1	B	61	TRP	C-N-CA	8.07	130.93	120.44
1	B	127	ARG	NH1-CZ-NH2	-8.05	108.83	119.30
1	A	111	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	B	90	LEU	N-CA-CB	-8.02	98.74	110.53
1	A	185	VAL	O-C-N	-7.99	114.08	121.91
1	B	162	GLN	CA-C-O	-7.99	111.74	120.36
1	B	130	VAL	CA-CB-CG1	7.97	123.95	110.40
1	B	223	GLU	N-CA-CB	7.88	120.56	110.23
1	B	64	GLN	CB-CG-CD	7.88	126.00	112.60
1	B	139	ASP	CA-CB-CG	7.86	120.46	112.60
1	B	2	LYS	CB-CG-CD	7.86	129.37	111.30
1	A	41	GLY	O-C-N	7.84	131.85	123.23
1	A	189	ALA	O-C-N	-7.84	113.81	122.12
1	B	6	GLU	CB-CG-CD	7.82	125.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	GLN	OE1-CD-NE2	7.77	130.37	122.60
1	B	187	MET	CA-C-O	-7.76	112.71	120.70
1	A	7	LEU	CA-C-O	-7.76	112.85	121.00
1	B	19	ASN	CA-C-O	-7.74	111.99	120.43
1	B	135	VAL	O-C-N	-7.74	114.31	121.89
1	A	48	LYS	N-CA-CB	7.73	124.67	110.99
1	A	6	GLU	N-CA-CB	7.69	121.54	110.16
1	B	193	ASP	CA-C-O	-7.67	112.68	121.65
1	A	37	ASN	CB-CG-ND2	7.66	127.89	116.40
1	B	217	HIS	O-C-N	-7.63	114.03	122.12
1	A	213	MET	N-CA-CB	7.63	121.07	110.01
1	A	6	GLU	CA-C-O	-7.62	112.35	120.42
1	A	76	ASN	N-CA-C	7.61	122.12	111.92
1	B	57	HIS	CA-CB-CG	-7.59	106.21	113.80
1	B	16	THR	CA-C-O	-7.58	112.39	120.80
1	B	199	PHE	CA-CB-CG	-7.55	106.25	113.80
1	B	107	ARG	CG-CD-NE	7.55	128.60	112.00
1	B	56	ILE	N-CA-CB	7.52	119.35	110.55
1	B	180	SER	CA-CB-OG	7.52	126.14	111.10
1	B	248	GLU	CB-CG-CD	7.48	125.32	112.60
1	B	14	GLU	CG-CD-OE2	-7.48	101.20	118.40
1	A	85	ASP	CA-C-N	7.45	133.17	120.72
1	A	85	ASP	C-N-CA	7.45	133.17	120.72
1	A	105	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	258	ILE	CA-C-O	-7.45	112.47	120.36
1	B	150	PHE	CA-CB-CG	7.41	121.21	113.80
1	B	19	ASN	N-CA-C	-7.41	97.17	109.24
1	B	198	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	11	VAL	CB-CA-C	7.39	122.42	112.22
1	B	211	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	B	107	ARG	CA-CB-CG	7.37	128.83	114.10
1	B	27	LEU	N-CA-C	-7.36	96.53	108.52
1	B	244	PHE	CA-CB-CG	-7.33	106.47	113.80
1	B	42	PHE	O-C-N	7.28	127.95	121.18
1	B	69	ILE	CA-C-O	-7.26	111.70	120.78
1	A	70	ALA	CA-C-O	-7.25	113.09	121.07
1	B	86	GLU	CA-CB-CG	7.25	128.59	114.10
1	A	96	LYS	N-CA-CB	-7.24	99.44	110.16
1	B	53	ARG	NH1-CZ-NH2	7.24	128.71	119.30
1	B	130	VAL	CB-CA-C	7.23	120.88	110.33
1	B	256	PRO	O-C-N	7.22	132.16	122.99
1	B	76	ASN	CA-CB-CG	7.22	119.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	LEU	N-CA-CB	7.18	121.82	110.55
1	B	244	PHE	N-CA-CB	-7.15	99.64	110.01
1	B	208	LEU	CA-C-O	-7.12	112.67	120.36
1	B	89	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	8	MET	CA-C-N	7.11	129.81	120.28
1	A	8	MET	C-N-CA	7.11	129.81	120.28
1	B	249	ILE	CA-CB-CG2	7.11	122.58	110.50
1	B	188	MET	CA-C-N	7.09	129.79	120.28
1	B	188	MET	C-N-CA	7.09	129.79	120.28
1	A	161	CYS	CA-C-O	-7.09	112.09	120.60
1	B	105	ASP	N-CA-C	7.08	125.88	110.80
1	B	225	ARG	CG-CD-NE	-7.08	96.43	112.00
1	A	48	LYS	CA-C-O	-7.07	112.09	120.43
1	A	211	ASN	OD1-CG-ND2	-7.04	115.56	122.60
1	A	24	THR	CA-C-O	-7.01	113.05	120.55
1	B	237	GLU	CG-CD-OE2	7.01	134.52	118.40
1	B	62	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	130	VAL	N-CA-C	-7.00	98.31	108.11
1	B	148	ALA	N-CA-C	6.99	121.94	113.41
1	A	60	LEU	CB-CA-C	6.99	122.39	110.79
1	A	54	SER	N-CA-C	-6.99	104.22	112.89
1	B	127	ARG	NE-CZ-NH2	-6.95	112.94	119.20
1	A	85	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	53	ARG	NE-CZ-NH2	-6.94	112.95	119.20
1	B	2	LYS	CA-C-N	6.94	129.58	120.28
1	B	2	LYS	C-N-CA	6.94	129.58	120.28
1	A	24	THR	N-CA-CB	6.93	120.38	110.13
1	B	188	MET	O-C-N	-6.92	114.94	122.07
1	B	121	ASN	OD1-CG-ND2	6.92	129.52	122.60
1	A	113	THR	CA-CB-CG2	6.91	122.25	110.50
1	A	234	ARG	N-CA-CB	-6.90	100.86	111.56
1	B	235	LYS	CA-C-O	6.88	125.28	119.71
1	A	114	THR	CA-CB-OG1	-6.87	99.30	109.60
1	B	108	HIS	N-CA-CB	6.86	122.34	110.81
1	B	211	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	114	THR	CA-C-O	-6.84	113.64	120.82
1	B	129	ILE	N-CA-C	6.84	119.38	108.85
1	B	244	PHE	CB-CA-C	6.83	121.61	110.88
1	B	1	MET	CB-CA-C	6.83	123.08	110.10
1	B	218	LEU	CA-C-N	6.83	129.73	120.44
1	B	218	LEU	C-N-CA	6.83	129.73	120.44
1	A	11	VAL	CA-CB-CG1	6.83	122.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ASN	CA-CB-CG	-6.83	105.78	112.60
1	A	50	CYS	CA-C-O	-6.82	113.40	121.11
1	A	188	MET	CA-C-O	-6.79	113.71	120.70
1	B	167	SER	CA-C-O	6.79	129.37	120.21
1	B	116	LEU	O-C-N	-6.77	115.05	122.09
1	B	230	LEU	CA-C-N	6.77	132.60	122.98
1	B	230	LEU	C-N-CA	6.77	132.60	122.98
1	B	127	ARG	CA-C-O	-6.76	113.36	121.34
1	B	57	HIS	CA-C-O	-6.75	113.40	120.55
1	B	81	ASP	N-CA-C	6.75	119.47	111.71
1	A	259	LYS	O-C-N	6.75	130.86	123.10
1	B	32	HIS	CA-CB-CG	-6.74	107.06	113.80
1	B	53	ARG	N-CA-C	6.72	118.61	111.28
1	A	84	ALA	CA-C-O	6.72	128.71	121.05
1	B	13	ASP	CA-CB-CG	6.71	119.31	112.60
1	B	257	GLY	CA-C-O	-6.71	113.52	122.24
1	A	42	PHE	CA-CB-CG	-6.70	107.10	113.80
1	A	83	TRP	CB-CA-C	6.67	124.00	110.38
1	A	20	ASP	CA-CB-CG	-6.67	105.93	112.60
1	B	17	GLN	CA-CB-CG	6.67	127.44	114.10
1	A	212	HIS	CA-CB-CG	6.65	120.45	113.80
1	B	21	ARG	NE-CZ-NH2	6.63	125.17	119.20
1	B	75	ASN	CA-CB-CG	6.63	119.23	112.60
1	B	90	LEU	CA-C-N	6.62	132.27	121.87
1	B	90	LEU	C-N-CA	6.62	132.27	121.87
1	B	239	ILE	CA-C-O	6.62	128.04	120.03
1	B	134	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	117	ASN	CB-CG-ND2	6.60	126.30	116.40
1	B	126	ARG	N-CA-C	-6.59	104.81	112.92
1	B	255	HIS	N-CA-C	-6.58	100.63	110.24
1	B	140	LYS	CA-CB-CG	6.57	127.25	114.10
1	A	57	HIS	O-C-N	6.57	129.09	122.12
1	B	234	ARG	NH1-CZ-NH2	6.56	127.83	119.30
1	A	113	THR	CB-CA-C	6.55	121.99	110.85
1	A	27	LEU	N-CA-C	-6.54	97.75	108.41
1	A	253	ASP	O-C-N	6.54	127.25	121.37
1	A	180	SER	CA-C-N	6.53	130.24	120.31
1	A	180	SER	C-N-CA	6.53	130.24	120.31
1	B	12	LEU	CA-C-N	6.53	129.56	120.29
1	B	12	LEU	C-N-CA	6.53	129.56	120.29
1	A	72	LEU	CA-C-N	6.52	128.92	120.44
1	A	72	LEU	C-N-CA	6.52	128.92	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	B	64	GLN	N-CA-CB	6.51	121.35	110.41
1	A	257	GLY	CA-C-N	6.50	132.03	122.99
1	A	257	GLY	C-N-CA	6.50	132.03	122.99
1	B	172	LEU	CA-C-O	-6.50	113.97	120.80
1	B	58	GLU	N-CA-CB	6.49	119.43	110.01
1	B	3	GLN	O-C-N	6.48	128.99	122.12
1	A	95	GLY	CA-C-O	-6.47	114.08	120.75
1	A	260	ALA	O-C-N	6.47	126.47	121.88
1	A	188	MET	CA-C-N	6.47	128.95	120.28
1	A	188	MET	C-N-CA	6.47	128.95	120.28
1	B	243	ARG	N-CA-CB	6.47	122.46	111.66
1	A	162	GLN	CA-C-O	-6.46	113.38	120.36
1	B	198	ASP	CB-CG-OD1	6.46	133.26	118.40
1	A	14	GLU	CA-C-O	-6.46	111.56	119.18
1	A	253	ASP	CA-C-O	-6.45	112.12	120.83
1	B	217	HIS	CA-C-O	6.45	127.39	120.55
1	A	262	VAL	CA-C-O	-6.45	113.42	120.71
1	B	111	GLN	CA-C-O	-6.45	112.55	119.97
1	B	153	TYR	N-CA-CB	-6.45	99.67	110.57
1	B	9	GLN	CA-C-O	6.44	127.25	120.42
1	B	58	GLU	N-CA-C	-6.41	104.21	111.07
1	B	202	THR	CA-C-N	-6.41	116.38	122.66
1	B	202	THR	C-N-CA	-6.41	116.38	122.66
1	B	183	LEU	CB-CA-C	6.41	120.94	110.88
1	A	71	TYR	O-C-N	6.41	128.91	122.12
1	B	96	LYS	CA-C-O	6.40	127.54	120.82
1	A	79	ILE	N-CA-C	6.40	119.05	111.05
1	B	13	ASP	N-CA-C	6.39	118.33	111.36
1	B	165	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	B	96	LYS	O-C-N	-6.39	115.49	122.07
1	B	105	ASP	CA-C-N	6.39	133.21	122.16
1	B	105	ASP	C-N-CA	6.39	133.21	122.16
1	A	190	GLN	OE1-CD-NE2	6.38	128.98	122.60
1	B	187	MET	CG-SD-CE	-6.38	86.87	100.90
1	B	163	LEU	CA-C-O	-6.37	113.96	120.71
1	A	202	THR	CA-CB-OG1	-6.37	100.05	109.60
1	A	223	GLU	CB-CA-C	6.36	117.13	109.31
1	B	256	PRO	CA-C-O	-6.35	114.32	121.43
1	B	249	ILE	CA-C-O	6.35	126.99	120.39
1	A	257	GLY	CA-C-O	6.34	130.81	122.31
1	A	6	GLU	CB-CG-CD	6.34	123.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	HIS	CA-CB-CG	6.34	120.14	113.80
1	A	13	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	230	LEU	CA-C-O	-6.33	113.53	120.43
1	B	126	ARG	NE-CZ-NH2	6.33	124.89	119.20
1	A	74	GLU	CG-CD-OE1	6.33	132.95	118.40
1	A	249	ILE	CA-CB-CG2	6.33	121.25	110.50
1	A	158	LYS	O-C-N	6.32	131.45	123.23
1	B	191	GLN	CA-C-O	6.32	127.24	120.10
1	B	207	HIS	CA-CB-CG	-6.32	107.48	113.80
1	A	99	ARG	NE-CZ-NH2	6.32	124.88	119.20
1	B	9	GLN	CA-C-N	6.32	128.74	120.28
1	B	9	GLN	C-N-CA	6.32	128.74	120.28
1	A	153	TYR	CA-C-O	-6.31	112.98	120.43
1	B	54	SER	N-CA-C	-6.31	104.50	111.82
1	B	126	ARG	NH1-CZ-NH2	-6.31	111.09	119.30
1	B	176	PHE	CA-C-N	6.30	129.24	120.29
1	B	176	PHE	C-N-CA	6.30	129.24	120.29
1	B	49	ARG	NH1-CZ-NH2	6.30	127.49	119.30
1	A	222	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	B	107	ARG	CB-CG-CD	6.30	125.78	111.30
1	A	21	ARG	CA-C-O	6.29	127.43	120.63
1	B	34	MET	CB-CA-C	6.29	123.92	110.07
1	B	36	PHE	CA-CB-CG	-6.29	107.51	113.80
1	B	28	SER	N-CA-C	6.29	118.97	109.23
1	B	64	GLN	CA-C-N	6.28	131.08	120.91
1	B	64	GLN	C-N-CA	6.28	131.08	120.91
1	A	127	ARG	N-CA-C	6.26	118.89	110.88
1	B	102	PRO	CB-CA-C	6.25	118.42	111.11
1	A	152	PHE	CA-CB-CG	-6.25	107.56	113.80
1	A	230	LEU	O-C-N	6.23	130.31	123.27
1	B	41	GLY	O-C-N	6.22	130.79	122.70
1	B	139	ASP	CB-CG-OD1	6.22	132.71	118.40
1	A	132	ALA	N-CA-C	-6.21	105.75	113.38
1	A	238	SER	CA-C-N	6.21	130.27	120.47
1	A	238	SER	C-N-CA	6.21	130.27	120.47
1	A	42	PHE	CB-CA-C	6.20	119.43	109.51
1	B	76	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	21	ARG	CA-C-N	6.19	133.64	121.58
1	B	21	ARG	C-N-CA	6.19	133.64	121.58
1	B	177	ASN	CA-C-O	-6.19	113.86	120.42
1	A	169	ASP	CA-C-N	6.18	128.92	120.46
1	A	169	ASP	C-N-CA	6.18	128.92	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	GLN	CA-C-O	-6.18	113.19	120.60
1	A	60	LEU	O-C-N	-6.17	115.58	122.12
1	A	4	TYR	CB-CG-CD2	6.16	130.04	120.80
1	B	42	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	21	ARG	N-CA-CB	-6.16	100.82	110.06
1	A	250	GLU	CB-CG-CD	6.15	123.06	112.60
1	B	77	VAL	N-CA-C	-6.15	99.44	108.54
1	A	188	MET	N-CA-C	-6.14	104.51	111.14
1	B	141	MET	CA-C-O	-6.14	114.05	121.05
1	B	10	LYS	N-CA-C	-6.12	104.61	111.28
1	A	10	LYS	CA-C-O	-6.12	113.94	120.42
1	A	113	THR	N-CA-CB	6.10	119.19	110.16
1	A	232	ILE	CB-CA-C	6.10	119.34	110.98
1	B	249	ILE	CB-CA-C	6.09	119.42	110.77
1	B	118	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	A	49	ARG	CD-NE-CZ	-6.07	115.90	124.40
1	B	67	THR	CB-CA-C	6.07	120.63	110.44
1	A	196	VAL	CB-CA-C	6.06	119.94	111.34
1	A	221	SER	CA-C-O	6.05	126.60	119.28
1	A	115	VAL	CA-C-N	6.05	128.30	120.44
1	A	115	VAL	C-N-CA	6.05	128.30	120.44
1	B	46	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	75	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	87	ASN	CB-CG-OD1	-6.04	108.72	120.80
1	B	246	ASP	CB-CG-OD2	6.04	132.28	118.40
1	A	158	LYS	CA-C-O	-6.03	114.19	120.70
1	A	109	ILE	N-CA-CB	-6.03	103.76	110.99
1	A	42	PHE	O-C-N	6.01	126.42	121.31
1	B	109	ILE	CA-C-N	6.01	131.67	122.77
1	B	109	ILE	C-N-CA	6.01	131.67	122.77
1	B	148	ALA	N-CA-CB	-5.99	101.73	110.47
1	A	241	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	263	ALA	CA-C-O	5.98	127.30	120.54
1	B	135	VAL	CB-CA-C	5.97	119.86	112.04
1	B	250	GLU	CG-CD-OE2	-5.97	104.67	118.40
1	B	50	CYS	CA-C-O	-5.97	114.37	121.11
1	A	240	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	105	ASP	N-CA-C	5.94	119.28	112.57
1	B	79	ILE	CA-C-O	-5.93	114.88	121.05
1	B	234	ARG	CD-NE-CZ	5.93	132.71	124.40
1	B	39	GLN	CA-CB-CG	5.93	125.96	114.10
1	B	176	PHE	N-CA-CB	5.93	118.66	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	THR	CA-CB-OG1	-5.92	100.71	109.60
1	A	129	ILE	CA-C-O	-5.92	114.04	120.67
1	A	165	GLN	CA-C-O	-5.91	114.14	120.46
1	B	72	LEU	CB-CA-C	5.91	120.90	110.85
1	B	222	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	B	241	ASP	O-C-N	5.91	130.01	122.39
1	A	118	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	B	96	LYS	CA-C-N	5.90	128.67	120.29
1	B	96	LYS	C-N-CA	5.90	128.67	120.29
1	A	211	ASN	CB-CG-OD1	5.90	132.60	120.80
1	A	120	LYS	CA-C-O	-5.89	113.70	120.24
1	A	20	ASP	CB-CA-C	5.89	124.45	111.09
1	B	142	ALA	CA-C-O	5.88	126.73	119.97
1	A	10	LYS	CB-CA-C	5.88	120.84	110.85
1	A	127	ARG	NH1-CZ-NH2	-5.87	111.66	119.30
1	B	170	VAL	CA-C-O	-5.86	115.02	121.29
1	A	246	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	126	ARG	NE-CZ-NH2	-5.85	113.93	119.20
1	A	249	ILE	CB-CA-C	5.85	119.55	110.83
1	A	77	VAL	CA-CB-CG2	-5.84	100.47	110.40
1	A	245	GLU	CB-CG-CD	5.84	122.53	112.60
1	B	121	ASN	CA-C-N	5.84	129.27	122.85
1	B	121	ASN	C-N-CA	5.84	129.27	122.85
1	B	76	ASN	CB-CA-C	5.83	120.73	111.23
1	A	101	TRP	N-CA-CB	-5.83	99.02	109.68
1	A	47	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	105	ASP	CA-C-N	5.82	130.34	120.91
1	A	105	ASP	C-N-CA	5.82	130.34	120.91
1	A	4	TYR	N-CA-CB	-5.82	101.58	110.01
1	B	186	HIS	CA-C-O	-5.81	114.72	120.82
1	A	206	THR	CA-C-O	-5.81	113.93	120.32
1	A	232	ILE	CA-C-N	5.81	132.55	122.56
1	A	232	ILE	C-N-CA	5.81	132.55	122.56
1	A	46	THR	CA-CB-OG1	-5.80	100.89	109.60
1	A	206	THR	CA-C-N	-5.80	113.08	122.36
1	A	206	THR	C-N-CA	-5.80	113.08	122.36
1	B	152	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	132	ALA	O-C-N	-5.80	114.82	122.42
1	B	90	LEU	O-C-N	-5.79	114.73	122.49
1	A	199	PHE	O-C-N	-5.78	116.63	123.22
1	A	258	ILE	CA-C-N	-5.78	112.81	122.64
1	A	258	ILE	C-N-CA	-5.78	112.81	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	MET	CA-C-O	-5.78	114.76	120.82
1	B	146	CYS	CA-C-N	5.77	131.58	122.34
1	B	146	CYS	C-N-CA	5.77	131.58	122.34
1	B	156	ASP	CA-C-O	-5.77	114.99	122.14
1	A	198	ASP	CB-CA-C	-5.76	98.83	109.37
1	B	215	GLN	CA-C-O	-5.76	114.44	120.55
1	B	14	GLU	OE1-CD-OE2	5.76	136.72	122.90
1	B	207	HIS	N-CA-C	5.75	117.93	109.24
1	A	243	ARG	N-CA-C	-5.74	100.78	109.85
1	B	17	GLN	CA-C-O	-5.74	113.79	120.62
1	B	183	LEU	CA-C-N	5.74	127.97	120.28
1	B	183	LEU	C-N-CA	5.74	127.97	120.28
1	A	5	LEU	CA-C-N	5.74	128.43	120.29
1	A	5	LEU	C-N-CA	5.74	128.43	120.29
1	A	1	MET	CG-SD-CE	5.73	113.52	100.90
1	A	148	ALA	N-CA-CB	-5.73	101.73	110.33
1	A	129	ILE	N-CA-C	5.73	117.00	108.46
1	B	86	GLU	CG-CD-OE1	5.73	131.57	118.40
1	B	48	LYS	N-CA-C	-5.73	98.93	108.32
1	B	224	PRO	N-CA-C	-5.72	102.28	111.38
1	A	94	TYR	N-CA-C	5.72	122.99	110.80
1	B	113	THR	CA-C-O	-5.72	114.81	120.82
1	A	1	MET	CB-CA-C	-5.70	99.26	110.10
1	B	100	ALA	CA-C-O	-5.70	111.95	122.62
1	A	149	PHE	N-CA-CB	-5.69	100.95	110.57
1	B	133	TRP	O-C-N	5.69	130.01	122.56
1	A	95	GLY	O-C-N	5.68	127.64	122.19
1	A	163	LEU	CA-C-N	5.68	131.18	123.11
1	A	163	LEU	C-N-CA	5.68	131.18	123.11
1	A	177	ASN	CB-CG-ND2	5.68	124.91	116.40
1	A	217	HIS	CA-CB-CG	-5.68	108.12	113.80
1	A	239	ILE	CA-CB-CG1	5.68	120.05	110.40
1	A	19	ASN	N-CA-C	-5.67	102.12	110.52
1	B	133	TRP	CA-C-O	-5.67	115.55	122.64
1	B	20	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	233	LYS	CA-CB-CG	5.67	125.43	114.10
1	A	190	GLN	CG-CD-OE1	-5.66	109.48	120.80
1	B	184	LEU	CA-C-O	-5.66	114.55	120.55
1	B	168	CYS	N-CA-C	5.65	117.64	108.26
1	B	54	SER	CA-C-O	-5.65	113.48	119.97
1	B	186	HIS	N-CA-CB	5.65	118.20	110.01
1	A	189	ALA	CA-C-N	5.64	128.30	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ALA	C-N-CA	5.64	128.30	120.29
1	A	2	LYS	CA-C-O	-5.63	114.88	120.90
1	B	129	ILE	O-C-N	5.62	128.93	123.03
1	B	187	MET	O-C-N	5.62	128.16	122.09
1	A	197	GLY	O-C-N	5.62	130.00	122.70
1	A	259	LYS	N-CA-CB	5.62	119.78	110.63
1	B	220	LEU	N-CA-CB	-5.61	100.78	110.32
1	B	205	ASP	CA-C-O	-5.59	114.59	121.02
1	A	16	THR	CA-CB-CG2	5.59	120.00	110.50
1	B	223	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	12	LEU	CA-C-N	5.58	130.12	120.58
1	A	12	LEU	C-N-CA	5.58	130.12	120.58
1	B	253	ASP	CB-CG-OD2	-5.58	105.57	118.40
1	B	9	GLN	OE1-CD-NE2	5.58	128.18	122.60
1	A	172	LEU	CA-C-O	-5.57	115.05	120.89
1	B	62	PHE	N-CA-CB	5.56	118.08	110.01
1	A	253	ASP	N-CA-CB	-5.56	103.04	111.21
1	A	85	ASP	CB-CA-C	5.56	123.69	111.30
1	A	186	HIS	CA-C-N	5.53	128.14	120.29
1	A	186	HIS	C-N-CA	5.53	128.14	120.29
1	A	186	HIS	N-CA-CB	5.53	118.24	110.12
1	B	18	LYS	CA-CB-CG	5.53	125.15	114.10
1	B	147	HIS	CA-C-O	-5.52	115.39	121.58
1	A	1	MET	CA-C-O	-5.52	111.41	120.80
1	A	86	GLU	CB-CG-CD	5.52	121.99	112.60
1	B	253	ASP	CB-CA-C	5.52	121.89	111.29
1	A	14	GLU	O-C-N	5.51	128.70	122.20
1	B	99	ARG	CA-C-O	5.50	125.63	119.41
1	B	195	GLU	CA-C-O	-5.50	114.95	121.66
1	B	249	ILE	O-C-N	-5.49	117.38	123.20
1	A	81	ASP	N-CA-C	5.48	120.42	111.37
1	A	78	THR	CB-CA-C	5.48	119.53	109.99
1	A	222	ARG	CG-CD-NE	-5.48	99.94	112.00
1	B	137	GLU	CG-CD-OE1	-5.48	105.80	118.40
1	A	219	GLN	OE1-CD-NE2	5.47	128.07	122.60
1	B	168	CYS	N-CA-CB	-5.46	101.86	110.77
1	A	169	ASP	N-CA-C	-5.46	98.84	108.23
1	B	202	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	225	ARG	NH1-CZ-NH2	-5.45	112.21	119.30
1	A	87	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	104	PRO	CA-C-N	5.45	131.22	122.83
1	A	104	PRO	C-N-CA	5.45	131.22	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	TYR	CA-C-N	5.44	128.02	120.29
1	B	71	TYR	C-N-CA	5.44	128.02	120.29
1	A	257	GLY	N-CA-C	-5.44	105.57	112.54
1	A	227	LEU	N-CA-CB	-5.44	101.42	110.02
1	A	83	TRP	CA-C-O	5.43	126.20	119.79
1	A	41	GLY	CA-C-O	-5.43	116.62	122.05
1	B	77	VAL	CB-CA-C	5.43	117.43	111.08
1	A	92	PRO	O-C-N	5.42	129.82	122.12
1	A	59	LEU	CB-CG-CD2	5.42	126.95	110.70
1	A	85	ASP	N-CA-C	-5.40	103.49	110.19
1	A	235	LYS	CA-CB-CG	-5.40	103.29	114.10
1	A	151	GLN	CA-C-O	-5.40	114.45	120.66
1	B	99	ARG	O-C-N	-5.39	114.70	122.36
1	A	4	TYR	CB-CG-CD1	-5.38	112.74	120.80
1	B	37	ASN	CA-C-O	-5.37	114.53	120.60
1	B	162	GLN	O-C-N	5.37	129.69	123.30
1	B	98	TRP	CA-CB-CG	5.37	123.79	113.60
1	B	184	LEU	CA-C-N	5.36	127.81	120.46
1	B	184	LEU	C-N-CA	5.36	127.81	120.46
1	B	173	GLY	CA-C-O	-5.36	111.24	120.57
1	A	52	LEU	CB-CA-C	5.36	120.54	110.63
1	B	33	GLN	CB-CG-CD	5.34	121.69	112.60
1	B	76	ASN	N-CA-CB	-5.32	104.64	112.78
1	A	225	ARG	CB-CA-C	5.32	117.24	109.48
1	B	80	TRP	CA-C-N	5.32	127.93	120.28
1	B	80	TRP	C-N-CA	5.32	127.93	120.28
1	B	206	THR	CA-CB-OG1	-5.31	101.63	109.60
1	A	207	HIS	N-CA-C	5.31	117.05	109.14
1	B	104	PRO	N-CA-C	-5.30	106.94	113.84
1	A	198	ASP	CB-CG-OD1	5.30	130.59	118.40
1	A	49	ARG	N-CA-C	5.30	117.90	109.96
1	B	198	ASP	OD1-CG-OD2	-5.30	110.19	122.90
1	A	225	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	A	152	PHE	N-CA-CB	5.29	118.81	110.56
1	A	83	TRP	CA-C-N	5.28	128.97	121.42
1	A	83	TRP	C-N-CA	5.28	128.97	121.42
1	B	131	SER	CA-C-O	-5.27	114.67	120.36
1	A	169	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	216	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	117	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	B	39	GLN	CA-C-N	5.26	131.84	121.58
1	B	39	GLN	C-N-CA	5.26	131.84	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	VAL	O-C-N	5.26	126.97	121.87
1	A	77	VAL	N-CA-CB	5.24	118.27	111.67
1	A	217	HIS	N-CA-CB	5.24	117.82	110.12
1	B	64	GLN	CA-C-O	5.22	125.80	119.11
1	A	87	ASN	OD1-CG-ND2	5.22	127.82	122.60
1	B	107	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	B	181	TYR	N-CA-CB	5.22	117.88	110.16
1	B	44	LEU	CB-CA-C	5.21	118.64	110.19
1	B	259	LYS	CA-C-O	5.21	126.92	120.92
1	A	5	LEU	CB-CA-C	5.21	119.71	110.85
1	A	55	ILE	CA-C-N	5.21	127.23	120.56
1	A	55	ILE	C-N-CA	5.21	127.23	120.56
1	B	249	ILE	CB-CG1-CD1	-5.21	102.86	113.80
1	A	181	TYR	N-CA-CB	5.21	118.35	110.28
1	A	59	LEU	CA-C-O	-5.20	114.91	120.42
1	B	66	ASP	CB-CA-C	5.20	118.22	109.48
1	B	172	LEU	CA-CB-CG	5.20	134.49	116.30
1	A	127	ARG	N-CA-CB	-5.19	103.82	111.51
1	A	210	SER	CA-CB-OG	-5.19	100.72	111.10
1	B	186	HIS	CA-CB-CG	5.19	118.99	113.80
1	A	86	GLU	CA-CB-CG	5.18	124.46	114.10
1	B	117	ASN	CA-C-O	-5.18	114.01	119.97
1	A	206	THR	O-C-N	5.17	129.38	123.27
1	A	9	GLN	N-CA-C	-5.17	105.64	111.28
1	B	36	PHE	CA-C-O	-5.17	114.77	120.30
1	B	72	LEU	CA-CB-CG	5.17	134.40	116.30
1	A	107	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	98	TRP	CA-C-O	-5.16	115.38	120.70
1	A	54	SER	CB-CA-C	5.16	120.77	109.99
1	A	198	ASP	OD1-CG-OD2	-5.16	110.53	122.90
1	B	82	GLU	CA-CB-CG	5.15	124.40	114.10
1	A	178	ILE	N-CA-CB	5.14	117.16	110.57
1	B	96	LYS	N-CA-C	5.14	116.57	111.07
1	B	71	TYR	N-CA-C	-5.14	105.11	111.33
1	B	11	VAL	N-CA-C	5.14	115.86	110.62
1	A	143	LEU	N-CA-CB	-5.13	102.20	110.81
1	B	116	LEU	CA-C-N	5.12	128.10	120.31
1	B	116	LEU	C-N-CA	5.12	128.10	120.31
1	A	74	GLU	OE1-CD-OE2	-5.12	110.61	122.90
1	A	72	LEU	CB-CA-C	5.12	119.29	110.79
1	B	48	LYS	CB-CA-C	5.12	118.54	109.89
1	A	75	ASN	CA-C-N	5.12	129.82	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ASN	C-N-CA	5.12	129.82	122.35
1	B	117	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	72	LEU	N-CA-CB	-5.11	102.61	110.12
1	B	185	VAL	CA-CB-CG1	5.11	119.08	110.40
1	B	243	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	B	195	GLU	CG-CD-OE2	5.10	130.13	118.40
1	B	42	PHE	CB-CA-C	5.10	118.23	109.82
1	B	91	GLY	N-CA-C	-5.09	101.95	112.34
1	A	209	TYR	CA-C-N	5.08	127.80	120.38
1	A	209	TYR	C-N-CA	5.08	127.80	120.38
1	B	46	THR	OG1-CB-CG2	5.08	119.46	109.30
1	A	220	LEU	CA-CB-CG	5.08	134.07	116.30
1	A	73	HIS	CB-CA-C	-5.07	102.92	110.88
1	A	202	THR	N-CA-CB	5.07	119.56	110.80
1	A	99	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	B	4	TYR	CB-CA-C	5.06	118.82	110.88
1	B	169	ASP	N-CA-C	-5.05	99.54	108.23
1	A	91	GLY	N-CA-C	-5.05	102.04	112.34
1	B	51	HIS	CA-C-O	-5.05	115.67	120.92
1	A	97	GLN	CG-CD-NE2	5.04	123.97	116.40
1	A	29	ILE	N-CA-C	-5.04	101.80	108.96
1	A	183	LEU	CA-C-N	5.04	126.99	120.44
1	A	183	LEU	C-N-CA	5.04	126.99	120.44
1	B	84	ALA	N-CA-CB	-5.04	102.79	110.45
1	A	3	GLN	CA-C-O	5.03	126.10	120.82
1	A	169	ASP	N-CA-CB	-5.03	102.95	110.24
1	B	95	GLY	CA-C-O	-5.03	111.83	120.57
1	A	201	TRP	CA-C-O	-5.02	114.96	120.43
1	A	14	GLU	CG-CD-OE1	-5.02	106.86	118.40
1	B	113	THR	CA-CB-OG1	-5.02	102.07	109.60
1	B	252	TYR	CA-C-N	-5.02	116.99	123.16
1	B	252	TYR	C-N-CA	-5.02	116.99	123.16
1	A	159	LEU	CA-C-N	5.01	131.74	122.92
1	A	159	LEU	C-N-CA	5.01	131.74	122.92
1	A	209	TYR	N-CA-C	-5.01	103.44	110.50

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

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Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	127	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	2153	0	2080	54	0
1	B	2153	0	2080	71	0
2	A	23	0	12	0	0
2	B	23	0	12	2	0
3	A	37	0	23	1	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	4229	119	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 14.

All (119) 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:A:215:GLN:HE21	1:A:215:GLN:H	1.18	0.91
1:B:183:LEU:HD22	1:B:187:MET:HE2	1.59	0.84
1:B:259:LYS:HB3	4:B:400:HOH:O	1.78	0.82
1:A:53:ARG:HG3	1:A:53:ARG:HH11	1.50	0.76
1:B:56:ILE:C	1:B:56:ILE:HD13	2.13	0.73
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:H	1:A:215:GLN:NE2	1.88	0.67
1:B:69:ILE:HG21	1:B:80:TRP:HB3	1.76	0.67
1:B:183:LEU:HD22	1:B:187:MET:CE	2.26	0.66
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:A:8:MET:HE3	1:A:220:LEU:HD13	1.81	0.61
1:B:41:GLY:HA2	1:B:229:LYS:HE3	1.82	0.61
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:1:MET:HE2	1:B:45:VAL:HG12	1.83	0.59
1:B:54:SER:HB2	3:B:266:F89:H17	1.84	0.58
1:A:5:LEU:HD23	1:A:8:MET:HE2	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: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:B:93:VAL:O	1:B:94:TYR:C	2.50	0.55
1:A:215:GLN:HE21	1:A:215:GLN:N	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:B:59:LEU:HD23	1:B:187:MET:HE1	1.90	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:59:LEU:CD2	1:B:187:MET:HE1	2.40	0.52
1:B:1:MET:HE2	1:B:45:VAL:CG1	2.40	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:B:215:GLN:H	1.59	0.49
1:B:39:GLN:NE2	1:B:158:LYS:HE3	2.27	0.49
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:A:1:MET:HE2	1:A:45:VAL:HG12	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:NH1	1:A:53:ARG:CG	2.77	0.47
1:A:136:GLY:HA2	1:B:109:ILE:CD1	2.44	0.47
1:A:8:MET:CE	1:A:220:LEU:HD13	2.43	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:H	1:B:2:LYS:HD2	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:54:SER:HB2	1:A:77:VAL:HG22	1.98	0.44
1:A:215:GLN:NE2	1:A:215:GLN:N	2.63	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:B:134:ASN:HD22	1:B:134:ASN:C	2.25	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:O	1:B:74:GLU:CG	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:HD23	1:A:116:LEU:HA	1.80	0.43
1:A:36:PHE:CE1	1:A:178:ILE:CD1	3.01	0.43
1:A:154:VAL:O	1:B:18:LYS:HE2	2.18	0.43
1:A:184:LEU:HD12	1:A:184:LEU:HA	1.89	0.43
1:A:58:GLU:O	1:A:61:TRP:HB3	2.19	0.43
1:A:49:ARG:HH11	1:A:49:ARG:HD2	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:252:TYR:CZ	1:B:254:PRO:HG3	2.55	0.41
1:B:174:LEU:HD12	1:B:174:LEU:HA	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: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
1:B:96:LYS:HZ3	1:B:102:PRO:HG3	1.86	0.40
1:A:169:ASP:OD1	1:A:169:ASP:C	2.62	0.40
1:B:79:ILE:HG23	1:B:80:TRP:N	2.36	0.40
3:B:266:F89:C9	3:B:266:F89:H14	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	263/265 (99%)	256 (97%)	5 (2%)	2 (1%)	16 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	263/265 (99%)	250 (95%)	10 (4%)	3 (1%)	11	8
All	All	526/530 (99%)	506 (96%)	15 (3%)	5 (1%)	12	9

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 ⓘ

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%)	208 (89%)	25 (11%)	6	4
1	B	233/233 (100%)	203 (87%)	30 (13%)	4	2
All	All	466/466 (100%)	411 (88%)	55 (12%)	5	3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	11	VAL
1	A	20	ASP
1	A	27	LEU
1	A	37	ASN
1	A	45	VAL
1	A	53	ARG
1	A	59	LEU
1	A	60	LEU
1	A	73	HIS
1	A	86	GLU

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Mol	Chain	Res	Type
1	A	105	ASP
1	A	107	ARG
1	A	113	THR
1	A	115	VAL
1	A	120	LYS
1	A	175	PRO
1	A	178	ILE
1	A	208	LEU
1	A	215	GLN
1	A	227	LEU
1	A	239	ILE
1	A	249	ILE
1	A	259	LYS
1	A	264	ILE
1	B	2	LYS
1	B	17	GLN
1	B	18	LYS
1	B	38	LEU
1	B	54	SER
1	B	56	ILE
1	B	64	GLN
1	B	69	ILE
1	B	71	TYR
1	B	77	VAL
1	B	89	ASP
1	B	96	LYS
1	B	116	LEU
1	B	120	LYS
1	B	127	ARG
1	B	130	VAL
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	230	LEU
1	B	231	ILE
1	B	233	LYS
1	B	234	ARG
1	B	237	GLU
1	B	243	ARG

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Mol	Chain	Res	Type
1	B	256	PRO
1	B	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	73	HIS
1	A	97	GLN
1	A	117	ASN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	186	HIS
1	A	190	GLN
1	A	215	GLN
1	B	19	ASN
1	B	57	HIS
1	B	117	ASN
1	B	121	ASN
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 oligosaccharides 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	A	265	-	25,25,25	2.01	6 (24%)	37,38,38	2.04	11 (29%)
3	F89	B	266	-	41,41,41	2.45	11 (26%)	56,60,60	4.72	21 (37%)
3	F89	A	266	-	41,41,41	2.24	11 (26%)	56,60,60	4.22	22 (39%)
2	DGP	B	265	-	25,25,25	1.61	7 (28%)	37,38,38	1.45	7 (18%)

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	A	265	-	-	0/10/22/22	0/3/3/3
3	F89	B	266	-	-	10/18/30/30	0/5/5/5
3	F89	A	266	-	-	6/18/30/30	0/5/5/5
2	DGP	B	265	-	-	0/10/22/22	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	266	F89	O1-CT	7.11	1.43	1.22
3	B	266	F89	CA-N	6.91	1.54	1.46
3	B	266	F89	O1-CT	6.54	1.41	1.22
3	A	266	F89	C1A-C1	6.15	1.60	1.47
3	B	266	F89	C1A-C1	5.59	1.59	1.47
2	A	265	DGP	C5'-C4'	5.57	1.68	1.51
3	B	266	F89	C19-N	5.18	1.52	1.47
3	A	266	F89	C19-N	4.84	1.52	1.47
2	A	265	DGP	O5'-C5'	-4.15	1.28	1.44
2	B	265	DGP	C6-N1	-3.86	1.31	1.38
3	A	266	F89	C-N	-3.62	1.32	1.36
3	A	266	F89	C1-N2	-3.40	1.32	1.37
2	A	265	DGP	C6-N1	-3.37	1.32	1.38
3	B	266	F89	CB-CG	3.30	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	266	F89	C3-N2	3.16	1.45	1.36
3	B	266	F89	C4A-N4	3.12	1.45	1.39
3	B	266	F89	OE2-CD	3.05	1.40	1.30
3	B	266	F89	C-N	-3.02	1.33	1.36
3	A	266	F89	C3-N2	3.00	1.45	1.36
2	B	265	DGP	C2'-C1'	2.91	1.60	1.52
3	A	266	F89	C4A-N4	2.86	1.44	1.39
3	A	266	F89	OE2-CD	2.72	1.39	1.30
2	A	265	DGP	C1'-N9	-2.70	1.41	1.48
3	A	266	F89	CA-CT	2.63	1.57	1.52
2	A	265	DGP	C2'-C3'	-2.53	1.46	1.52
3	A	266	F89	CG-CD	2.50	1.56	1.50
3	B	266	F89	C13-N12	2.43	1.45	1.38
2	B	265	DGP	P-OP1	-2.35	1.43	1.50
2	A	265	DGP	C2'-C1'	2.22	1.58	1.52
2	B	265	DGP	P-OP2	-2.21	1.46	1.54
3	B	266	F89	CB-CA	2.19	1.57	1.53
2	B	265	DGP	C2-N2	-2.19	1.29	1.34
3	A	266	F89	C10-C9	2.14	1.42	1.37
2	B	265	DGP	O6-C6	2.07	1.27	1.23
2	B	265	DGP	P-OP3	-2.07	1.47	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	F89	C19-N-CA	-16.88	107.61	123.68
3	B	266	F89	C19-N-CA	-15.56	108.87	123.68
3	B	266	F89	O-C-N	15.19	137.40	125.34
3	A	266	F89	CA-N-C	13.45	142.39	121.86
3	B	266	F89	CA-N-C	12.79	141.38	121.86
3	A	266	F89	O-C-N	12.13	134.97	125.34
3	B	266	F89	C19-C15-C16	-9.25	103.92	109.73
3	B	266	F89	C15-C19-N	8.57	106.87	102.31
3	A	266	F89	C4A-N4-C3	8.35	126.48	118.16
3	B	266	F89	C19-N-C	-8.12	109.73	113.15
3	A	266	F89	C19-N-C	-7.48	110.00	113.15
3	B	266	F89	O2-CT-CA	6.87	135.76	113.34
3	B	266	F89	CB-CA-CT	6.84	127.13	112.14
3	A	266	F89	O-C-C16	-6.79	115.50	128.66
3	B	266	F89	O-C-C16	-6.57	115.93	128.66
3	B	266	F89	C4A-N4-C3	6.41	124.55	118.16
3	B	266	F89	C15-C16-C	6.07	112.23	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	265	DGP	O5'-P-OP1	5.67	121.77	106.44
3	B	266	F89	CG-CB-CA	-5.53	101.85	112.83
3	A	266	F89	C16-C-N	4.89	109.53	106.42
2	A	265	DGP	N2-C2-N1	4.64	126.55	116.76
3	B	266	F89	C1B-C1A-C1	4.58	126.22	121.28
3	A	266	F89	C1B-C1A-C1	4.36	125.99	121.28
3	B	266	F89	O1-CT-CA	-4.28	109.30	122.44
2	B	265	DGP	O6-C6-N1	-4.08	112.44	120.11
3	B	266	F89	O2-CT-O1	-4.05	114.89	124.08
3	A	266	F89	OE2-CD-OE1	3.82	133.17	123.33
3	A	266	F89	CB-CG-CD	-3.59	102.92	112.49
3	B	266	F89	C1-N2-C3	-3.54	121.94	123.87
2	A	265	DGP	C2-N1-C6	3.50	131.47	125.11
3	A	266	F89	C15-C19-N	3.43	104.13	102.31
3	A	266	F89	O1-CT-CA	-3.39	112.02	122.44
3	A	266	F89	N2-C3-N4	-3.34	117.87	123.15
2	A	265	DGP	C3'-C2'-C1'	-3.29	94.55	102.60
3	A	266	F89	O2-CT-CA	3.29	124.07	113.34
3	A	266	F89	C13-C14-C15	-3.27	116.39	120.88
3	A	266	F89	C19-C15-C16	-3.08	107.79	109.73
3	A	266	F89	C14-C13-N12	-3.02	112.66	120.78
2	A	265	DGP	O4'-C4'-C5'	-2.98	99.78	109.33
2	B	265	DGP	C3'-C2'-C1'	-2.89	95.52	102.60
3	A	266	F89	C3M-C3-N2	2.89	122.27	116.27
3	A	266	F89	C11-N12-C13	2.86	131.04	121.87
3	B	266	F89	O1A-C1-N2	-2.85	117.24	120.62
2	A	265	DGP	O6-C6-N1	-2.82	114.81	120.11
2	A	265	DGP	O6-C6-C5	2.81	133.96	126.53
3	B	266	F89	C1A-C1-N2	2.76	118.28	115.17
3	B	266	F89	C13-C14-C15	-2.67	117.21	120.88
2	A	265	DGP	O4'-C1'-N9	-2.63	103.19	107.86
2	A	265	DGP	N2-C2-N3	-2.61	114.57	119.67
3	B	266	F89	C3M-C3-N2	2.59	121.66	116.27
2	B	265	DGP	O4'-C4'-C3'	-2.47	100.02	105.65
2	A	265	DGP	N1-C2-N3	-2.45	118.84	123.32
3	B	266	F89	C19-C15-C14	2.36	134.13	128.32
2	B	265	DGP	O6-C6-C5	2.36	132.76	126.53
3	A	266	F89	C5-C4A-N4	2.33	121.57	118.61
3	A	266	F89	C18-C13-N12	2.09	125.69	120.96
2	B	265	DGP	C2-N1-C6	-2.07	121.36	125.11
2	B	265	DGP	O3'-C3'-C2'	-2.06	103.73	110.88
3	A	266	F89	C1A-C1-N2	2.03	117.45	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	265	DGP	N1-C2-N3	2.01	127.00	123.32
2	A	265	DGP	O4'-C4'-C3'	-2.00	101.08	105.65

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	266	F89	CT-CA-CB-CG
3	B	266	F89	CB-CA-N-C19
3	B	266	F89	CB-CA-N-C
3	B	266	F89	CB-CA-CT-O1
3	B	266	F89	N-CA-CB-CG
3	B	266	F89	CT-CA-CB-CG
3	B	266	F89	CB-CA-CT-O2
3	B	266	F89	CA-CB-CG-CD
3	A	266	F89	CA-CB-CG-CD
3	B	266	F89	CT-CA-N-C19
3	B	266	F89	N-CA-CT-O1
3	B	266	F89	N-CA-CT-O2
3	A	266	F89	CB-CA-N-C
3	A	266	F89	CB-CA-N-C19
3	A	266	F89	C9-C11-N12-C13
3	A	266	F89	N-CA-CB-CG

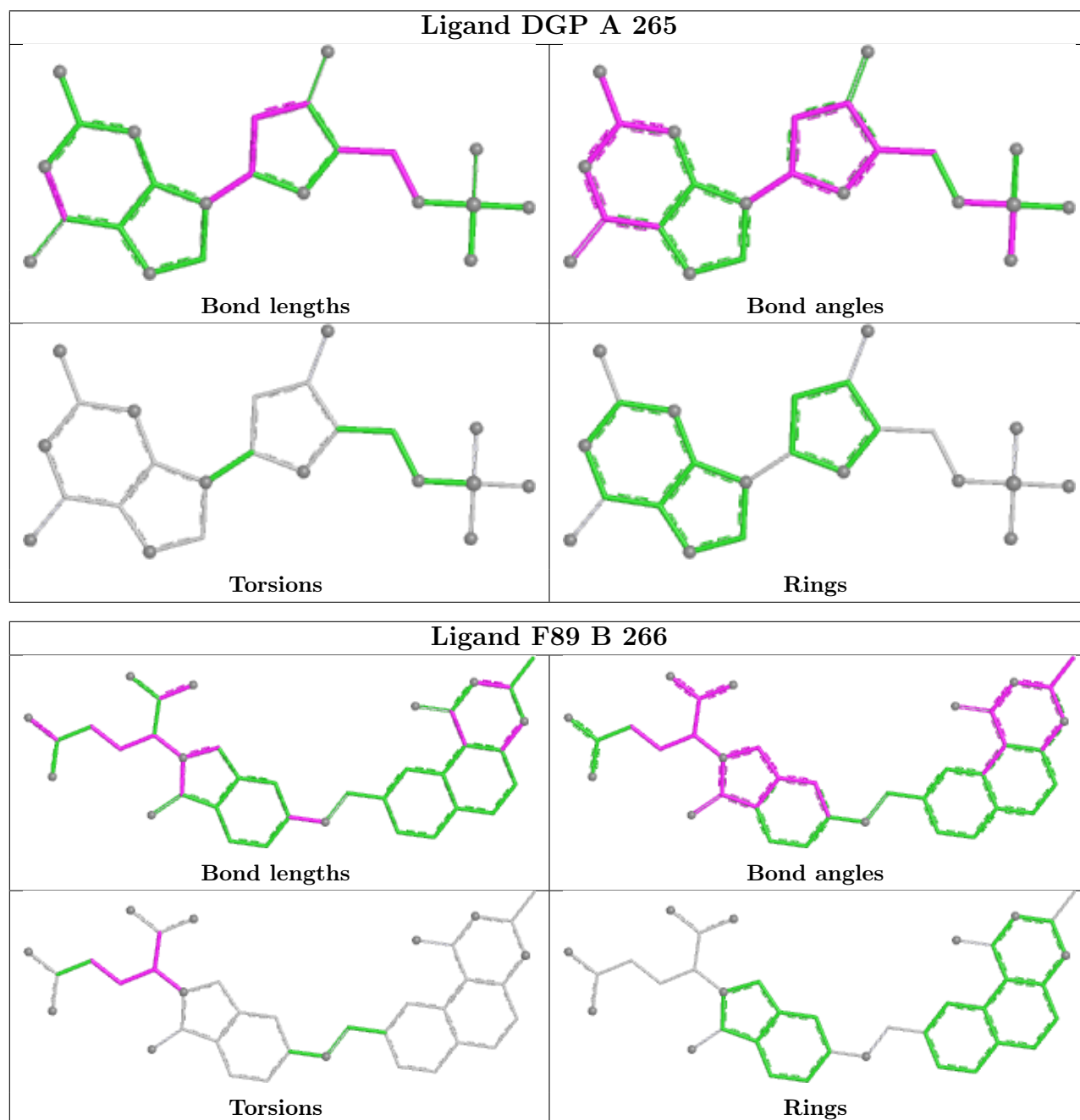
There are no ring outliers.

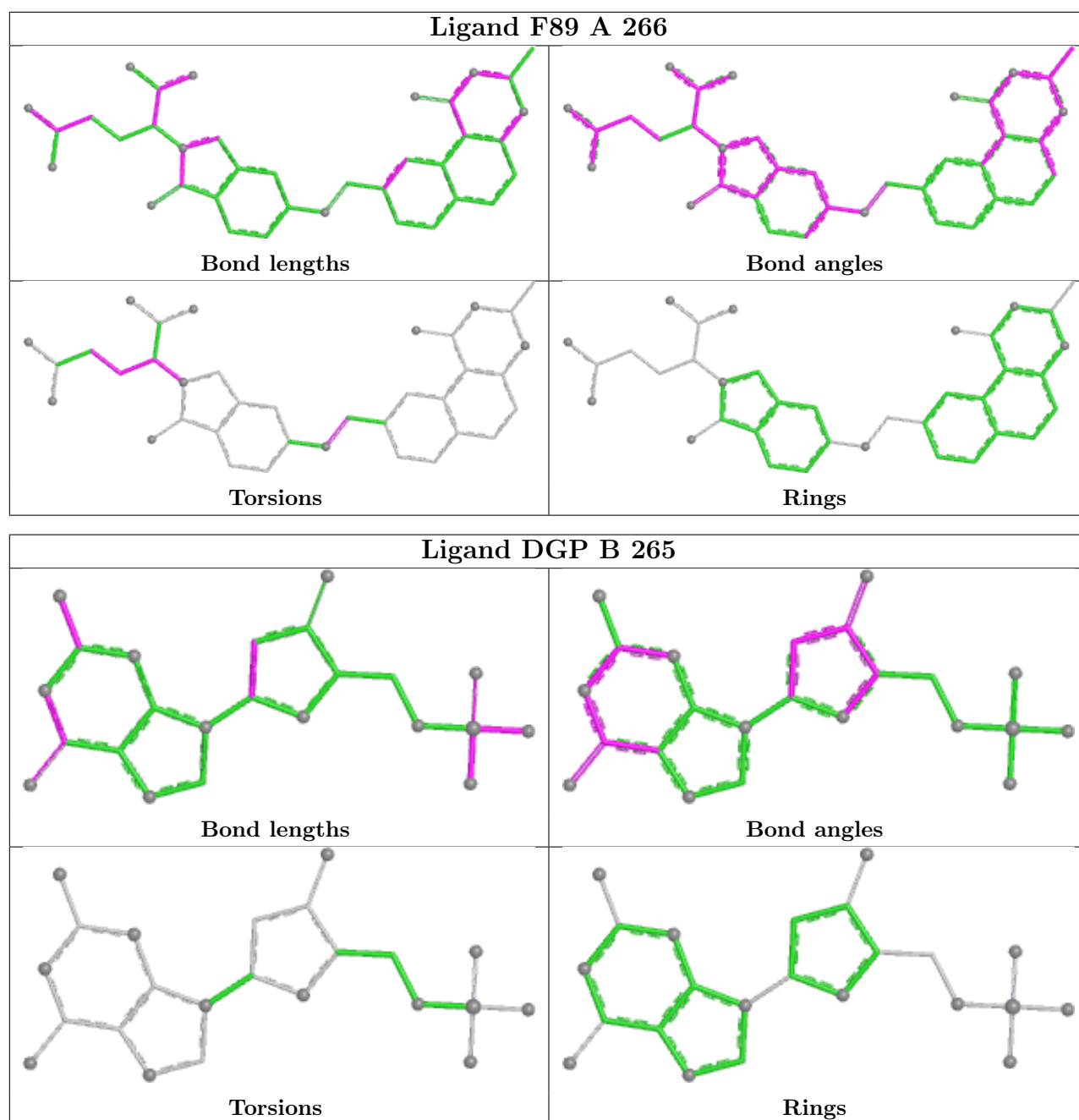
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	266	F89	5	0
3	A	266	F89	1	0
2	B	265	DGP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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 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.