



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:54 AM UTC

PDB ID : 2TSC / pdb_00002tsc
Title : STRUCTURE, MULTIPLE SITE BINDING, AND SEGMENTAL ACCOMMODATION IN THYMIDYLATE SYNTHASE ON BINDING D/UMP AND AN ANTI-FOLATE
Authors : Montfort, W.R.; Stroud, R.M.
Deposited on : 1991-07-03
Resolution : 1.97 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

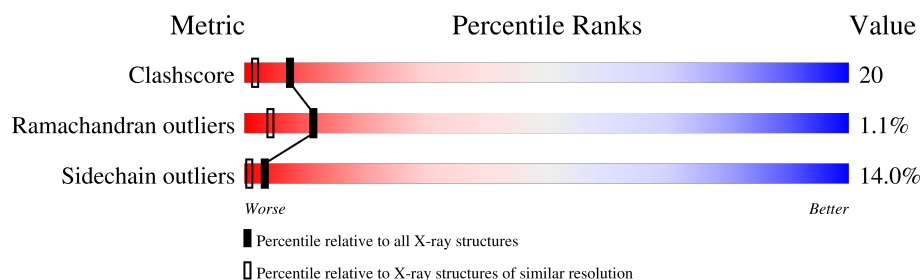
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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	264	27% 46% 21% 6%
1	B	264	30% 39% 21% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4600 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.

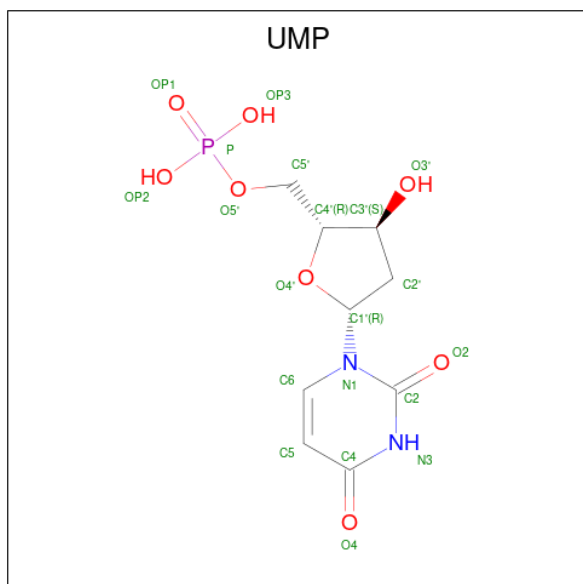
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2146	1371	370	393	12			
1	B	264	Total	C	N	O	S	0	0	0
			2146	1371	370	393	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ALA	LYS	conflict	UNP P0A884
B	235	ALA	LYS	conflict	UNP P0A884

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



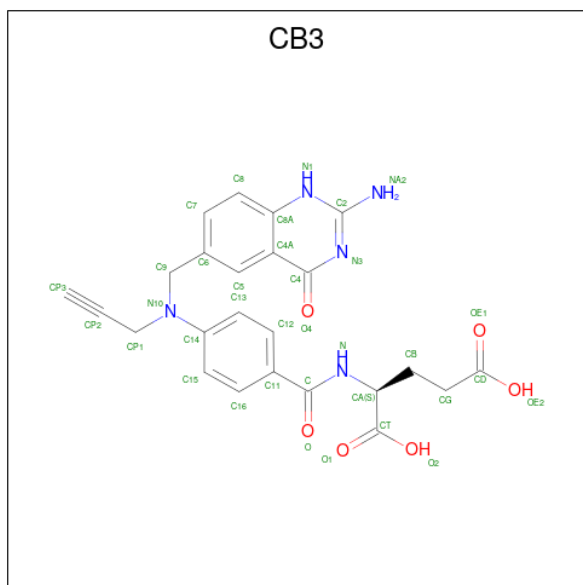
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is water.

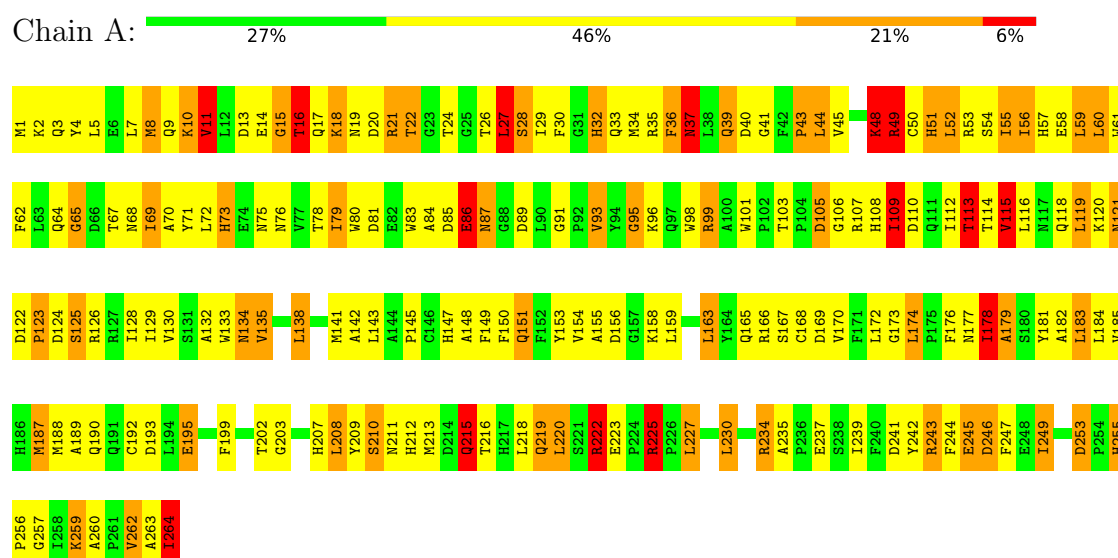
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	85	Total	O	0	0
			85	85		

3 Residue-property plots

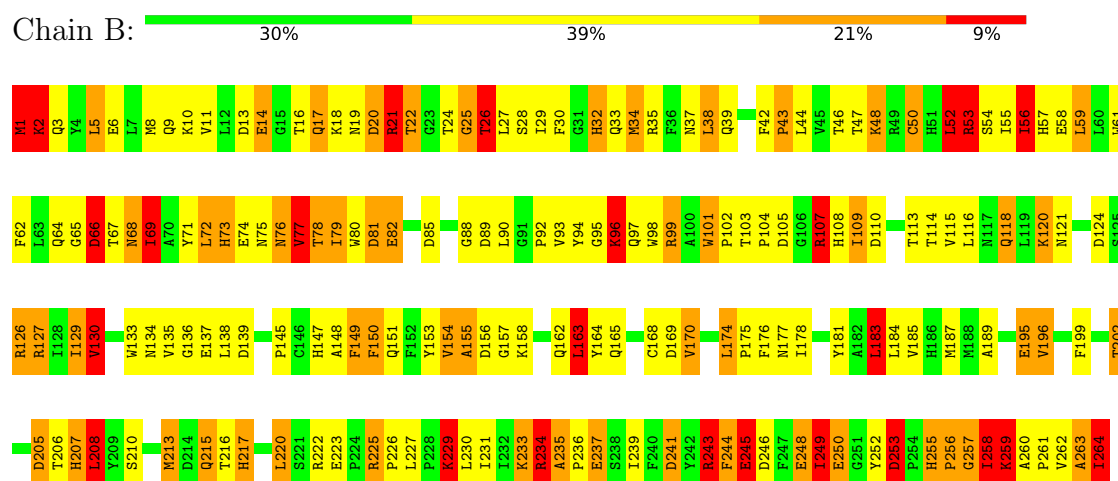
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	127.10 Å 127.10 Å 67.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 – 1.97	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-1.97)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: CB3, UMP

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	1.52	4/2206 (0.2%)	2.99	287/2996 (9.6%)
1	B	1.47	10/2206 (0.5%)	3.12	290/2996 (9.7%)
All	All	1.50	14/4412 (0.3%)	3.05	577/5992 (9.6%)

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	5
1	B	0	3
All	All	0	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	GLY	CA-C	-7.26	1.41	1.51
1	A	130	VAL	C-N	-7.25	1.23	1.33
1	B	257	GLY	N-CA	-7.00	1.35	1.45
1	B	264	ILE	N-CA	6.07	1.57	1.46
1	B	255	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	37	ASN	C-O	5.79	1.31	1.24
1	A	159	LEU	CA-CB	5.69	1.61	1.53
1	B	129	ILE	CA-CB	5.57	1.63	1.55
1	B	168	CYS	C-O	5.55	1.30	1.24
1	B	32	HIS	C-O	-5.39	1.17	1.23
1	B	102	PRO	C-O	5.09	1.27	1.24
1	B	163	LEU	C-O	-5.08	1.17	1.24
1	B	127	ARG	CZ-NH2	5.06	1.40	1.33
1	A	156	ASP	N-CA	5.04	1.52	1.46

All (577) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	GLY	N-CA-C	21.52	164.17	113.18
1	B	127	ARG	NE-CZ-NH1	19.79	141.29	121.50
1	B	253	ASP	N-CA-CB	18.64	137.48	111.20
1	B	127	ARG	NE-CZ-NH2	-16.44	104.40	119.20
1	A	19	ASN	OD1-CG-ND2	16.32	138.92	122.60
1	B	150	PHE	CA-CB-CG	15.70	129.50	113.80
1	B	99	ARG	NE-CZ-NH1	-14.14	107.36	121.50
1	B	33	GLN	OE1-CD-NE2	-13.50	109.10	122.60
1	A	35	ARG	CD-NE-CZ	13.05	142.67	124.40
1	B	241	ASP	CA-CB-CG	13.00	125.60	112.60
1	A	124	ASP	CA-C-O	-12.52	103.79	119.31
1	B	62	PHE	CA-CB-CG	12.28	126.08	113.80
1	A	19	ASN	CA-CB-CG	-12.03	100.57	112.60
1	B	130	VAL	N-CA-CB	11.88	127.98	111.82
1	A	262	VAL	CB-CA-C	-11.81	94.09	111.68
1	B	20	ASP	N-CA-CB	-11.69	91.75	110.46
1	B	253	ASP	O-C-N	11.49	131.78	121.32
1	B	48	LYS	N-CA-CB	11.40	131.17	110.99
1	A	13	ASP	CA-CB-CG	11.38	123.98	112.60
1	A	263	ALA	CA-C-N	11.27	141.98	121.70
1	A	263	ALA	C-N-CA	11.27	141.98	121.70
1	B	76	ASN	OD1-CG-ND2	11.25	133.85	122.60
1	B	56	ILE	CA-CB-CG2	11.01	129.22	110.50
1	B	37	ASN	CB-CA-C	10.83	128.31	110.22
1	B	223	GLU	N-CA-CB	10.80	126.53	109.90
1	B	64	GLN	CB-CG-CD	10.80	130.95	112.60
1	B	48	LYS	CA-CB-CG	10.69	135.48	114.10
1	B	26	THR	N-CA-CB	-10.67	93.84	111.66
1	B	148	ALA	N-CA-C	10.49	126.24	113.23
1	A	49	ARG	CD-NE-CZ	-10.46	109.75	124.40
1	B	127	ARG	CD-NE-CZ	10.46	139.04	124.40
1	B	155	ALA	CA-C-O	-10.35	105.71	120.51
1	B	32	HIS	CA-CB-CG	-10.35	103.45	113.80
1	B	59	LEU	CA-C-O	-10.31	109.49	120.42
1	B	9	GLN	OE1-CD-NE2	10.21	132.81	122.60
1	A	41	GLY	CA-C-O	-10.11	111.94	122.05
1	A	222	ARG	NE-CZ-NH1	10.10	131.60	121.50
1	B	130	VAL	CA-CB-CG1	10.04	127.46	110.40
1	A	68	ASN	OD1-CG-ND2	-10.01	112.59	122.60
1	B	121	ASN	OD1-CG-ND2	10.00	132.60	122.60
1	A	148	ALA	N-CA-C	9.97	123.96	111.69
1	A	75	ASN	CA-CB-CG	-9.87	102.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LEU	CA-C-O	-9.84	109.71	120.43
1	B	210	SER	CA-C-O	-9.75	110.22	120.55
1	A	215	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	A	177	ASN	CA-C-O	-9.53	110.81	120.82
1	A	168	CYS	N-CA-C	9.51	124.94	108.02
1	A	48	LYS	CA-C-O	-9.50	110.35	120.99
1	B	35	ARG	NE-CZ-NH1	9.48	130.98	121.50
1	A	56	ILE	CA-C-O	-9.46	110.55	121.05
1	A	125	SER	N-CA-CB	9.45	123.78	110.26
1	A	230	LEU	O-C-N	9.41	133.90	123.27
1	B	57	HIS	CA-CB-CG	-9.39	104.41	113.80
1	B	257	GLY	CA-C-N	9.38	138.85	121.97
1	B	257	GLY	C-N-CA	9.38	138.85	121.97
1	B	76	ASN	CA-CB-CG	-9.37	103.23	112.60
1	A	227	LEU	CB-CA-C	9.35	124.11	109.42
1	B	229	LYS	CA-C-O	-9.35	110.80	120.71
1	B	2	LYS	N-CA-CB	9.34	123.86	109.94
1	B	79	ILE	N-CA-C	9.21	120.03	110.36
1	A	234	ARG	NE-CZ-NH1	-9.20	112.30	121.50
1	B	184	LEU	CA-C-N	9.20	132.46	120.60
1	B	184	LEU	C-N-CA	9.20	132.46	120.60
1	B	6	GLU	CA-C-O	-9.13	110.87	120.55
1	A	35	ARG	NE-CZ-NH2	9.10	127.39	119.20
1	A	17	GLN	CB-CG-CD	-9.08	97.16	112.60
1	A	108	HIS	CA-C-O	-9.04	110.28	120.32
1	B	81	ASP	O-C-N	9.04	131.70	122.12
1	A	125	SER	CA-CB-OG	-9.02	93.05	111.10
1	B	56	ILE	N-CA-CB	8.99	121.07	110.55
1	A	11	VAL	CA-CB-CG1	8.98	125.67	110.40
1	A	234	ARG	CA-CB-CG	8.88	131.86	114.10
1	B	81	ASP	CA-C-O	-8.86	111.16	120.55
1	A	11	VAL	N-CA-CB	8.84	122.56	110.54
1	B	77	VAL	N-CA-CB	8.80	121.51	111.21
1	B	52	LEU	N-CA-C	8.80	123.27	112.54
1	A	36	PHE	CA-C-O	-8.79	110.93	120.24
1	B	68	ASN	CA-CB-CG	-8.75	103.85	112.60
1	B	223	GLU	CB-CA-C	-8.66	98.65	109.31
1	A	41	GLY	O-C-N	8.63	132.73	123.23
1	A	14	GLU	CA-C-N	8.56	129.77	120.44
1	A	14	GLU	C-N-CA	8.56	129.77	120.44
1	A	60	LEU	CA-C-N	8.52	131.51	120.44
1	A	60	LEU	C-N-CA	8.52	131.51	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	N-CA-CB	-8.46	95.93	110.32
1	A	68	ASN	CB-CG-ND2	8.44	129.06	116.40
1	B	72	LEU	CA-C-O	-8.43	112.02	120.70
1	A	138	LEU	CB-CA-C	8.39	124.95	110.68
1	B	64	GLN	N-CA-CB	8.32	123.95	110.40
1	A	58	GLU	CA-C-O	-8.31	111.74	120.55
1	A	67	THR	CA-CB-CG2	8.31	124.63	110.50
1	A	116	LEU	CA-C-O	-8.31	111.74	120.55
1	A	108	HIS	O-C-N	8.29	133.01	123.31
1	A	129	ILE	CA-C-N	8.29	134.51	122.99
1	A	129	ILE	C-N-CA	8.29	134.51	122.99
1	A	156	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	40	ASP	N-CA-CB	8.28	123.89	110.40
1	A	57	HIS	CA-CB-CG	-8.28	105.52	113.80
1	B	50	CYS	CB-CA-C	8.27	123.37	109.48
1	B	78	THR	N-CA-CB	-8.23	98.31	110.49
1	A	27	LEU	N-CA-C	-8.22	95.12	108.52
1	B	32	HIS	CA-C-O	-8.21	111.53	121.06
1	B	44	LEU	CA-C-O	-8.21	111.48	120.43
1	B	56	ILE	CA-C-O	-8.17	112.51	121.17
1	B	2	LYS	CA-C-O	-8.15	112.17	120.90
1	B	165	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	A	178	ILE	CA-CB-CG2	8.10	124.27	110.50
1	B	99	ARG	NH1-CZ-NH2	8.09	129.81	119.30
1	B	1	MET	CA-C-N	8.07	131.44	120.54
1	B	1	MET	C-N-CA	8.07	131.44	120.54
1	A	87	ASN	OD1-CG-ND2	8.06	130.66	122.60
1	A	134	ASN	CA-C-N	8.04	131.87	120.53
1	A	134	ASN	C-N-CA	8.04	131.87	120.53
1	B	210	SER	O-C-N	8.04	130.64	122.12
1	B	52	LEU	N-CA-CB	-8.03	97.05	110.39
1	B	34	MET	CB-CA-C	8.02	127.37	109.56
1	B	76	ASN	CA-C-O	-8.01	110.96	120.57
1	B	149	PHE	N-CA-CB	-8.01	97.48	110.77
1	A	112	ILE	CA-C-O	-8.00	111.90	121.18
1	A	35	ARG	NH1-CZ-NH2	-8.00	108.90	119.30
1	A	130	VAL	CA-C-N	7.92	134.16	122.99
1	A	130	VAL	C-N-CA	7.92	134.16	122.99
1	B	196	VAL	N-CA-CB	7.90	121.09	110.26
1	B	66	ASP	CA-CB-CG	-7.88	104.72	112.60
1	A	101	TRP	O-C-N	7.88	128.51	121.18
1	B	207	HIS	O-C-N	7.84	132.65	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	LEU	CA-C-O	-7.82	110.67	120.28
1	A	15	GLY	CA-C-O	-7.79	112.11	122.24
1	A	190	GLN	CG-CD-NE2	7.77	128.06	116.40
1	A	108	HIS	CA-CB-CG	-7.77	106.03	113.80
1	B	202	THR	CA-C-N	-7.74	115.59	122.47
1	B	202	THR	C-N-CA	-7.74	115.59	122.47
1	A	128	ILE	O-C-N	7.72	132.22	122.57
1	A	151	GLN	OE1-CD-NE2	-7.70	114.91	122.60
1	A	141	MET	CA-C-O	-7.68	111.86	120.54
1	B	59	LEU	O-C-N	7.68	130.90	122.15
1	A	247	PHE	CA-CB-CG	7.67	121.47	113.80
1	A	79	ILE	CA-C-O	7.64	129.27	120.03
1	B	195	GLU	CA-C-O	-7.63	112.20	121.36
1	B	207	HIS	N-CA-C	7.63	120.76	109.24
1	A	234	ARG	NE-CZ-NH2	7.62	126.05	119.20
1	B	244	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	59	LEU	CA-C-N	7.58	130.44	120.28
1	A	59	LEU	C-N-CA	7.58	130.44	120.28
1	B	109	ILE	N-CA-CB	7.58	121.87	111.41
1	A	173	GLY	N-CA-C	7.56	121.63	112.49
1	B	35	ARG	CA-C-O	-7.53	111.97	120.32
1	A	32	HIS	CA-C-O	-7.52	113.20	121.33
1	A	98	TRP	CA-C-O	7.51	128.71	120.82
1	A	115	VAL	CB-CA-C	7.51	122.59	112.22
1	A	257	GLY	CA-C-O	-7.50	113.16	121.71
1	A	61	TRP	CA-CB-CG	7.50	127.84	113.60
1	A	53	ARG	NE-CZ-NH1	7.49	128.99	121.50
1	B	243	ARG	CD-NE-CZ	7.48	134.88	124.40
1	A	176	PHE	CA-CB-CG	7.48	121.28	113.80
1	B	256	PRO	CA-C-N	7.47	136.04	121.41
1	B	256	PRO	C-N-CA	7.47	136.04	121.41
1	B	37	ASN	CA-CB-CG	-7.44	105.16	112.60
1	B	130	VAL	CB-CA-C	7.43	120.45	110.42
1	B	55	ILE	O-C-N	7.40	129.46	121.83
1	B	113	THR	O-C-N	7.38	130.56	122.15
1	B	223	GLU	CA-CB-CG	7.38	128.85	114.10
1	A	145	PRO	CA-C-O	-7.38	113.28	121.32
1	A	210	SER	CA-CB-OG	-7.37	96.37	111.10
1	B	195	GLU	N-CA-CB	-7.33	98.45	110.41
1	A	176	PHE	CA-C-N	7.31	129.94	120.44
1	A	176	PHE	C-N-CA	7.31	129.94	120.44
1	B	77	VAL	CA-C-O	7.31	128.56	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ALA	O-C-N	7.31	126.97	121.85
1	A	22	THR	CA-CB-OG1	-7.24	98.73	109.60
1	A	173	GLY	CA-C-O	-7.23	112.81	120.90
1	B	19	ASN	N-CA-C	-7.22	97.47	108.96
1	B	72	LEU	O-C-N	7.22	129.89	122.09
1	A	174	LEU	N-CA-C	7.22	122.64	113.25
1	A	177	ASN	O-C-N	7.22	129.51	122.07
1	A	154	VAL	CA-C-O	-7.22	112.71	120.36
1	B	234	ARG	N-CA-CB	7.20	124.22	111.69
1	B	183	LEU	CA-C-O	-7.20	113.28	120.70
1	A	20	ASP	CA-CB-CG	-7.19	105.41	112.60
1	B	199	PHE	CA-C-N	7.17	132.08	122.90
1	B	199	PHE	C-N-CA	7.17	132.08	122.90
1	B	28	SER	N-CA-CB	-7.17	98.32	111.37
1	A	151	GLN	CA-C-N	7.15	134.80	122.64
1	A	151	GLN	C-N-CA	7.15	134.80	122.64
1	A	234	ARG	CB-CG-CD	-7.14	94.88	111.30
1	A	109	ILE	CB-CG1-CD1	7.13	128.77	113.80
1	A	108	HIS	CA-C-N	-7.12	114.36	123.19
1	A	108	HIS	C-N-CA	-7.12	114.36	123.19
1	B	77	VAL	CB-CA-C	7.12	120.73	110.98
1	B	155	ALA	CA-C-N	-7.09	113.29	122.79
1	B	155	ALA	C-N-CA	-7.09	113.29	122.79
1	B	78	THR	CA-CB-OG1	-7.05	99.03	109.60
1	A	126	ARG	CA-C-N	7.01	133.50	122.49
1	A	126	ARG	C-N-CA	7.01	133.50	122.49
1	B	239	ILE	CA-CB-CG1	7.01	122.32	110.40
1	A	56	ILE	O-C-N	7.01	129.19	121.90
1	B	233	LYS	CA-C-O	-7.01	113.12	120.55
1	A	61	TRP	CA-C-O	-7.01	113.46	120.82
1	A	216	THR	CA-C-O	-7.00	113.47	120.82
1	A	48	LYS	N-CA-CB	7.00	124.53	111.52
1	B	174	LEU	CB-CA-C	6.99	123.95	110.17
1	A	149	PHE	N-CA-CB	-6.99	98.62	110.99
1	A	138	LEU	N-CA-CB	-6.99	99.58	110.06
1	A	255	HIS	N-CA-CB	6.99	119.33	110.04
1	B	195	GLU	CA-CB-CG	6.97	128.04	114.10
1	A	8	MET	CA-C-N	6.96	129.60	120.28
1	A	8	MET	C-N-CA	6.96	129.60	120.28
1	A	85	ASP	CA-C-N	6.95	130.29	120.28
1	A	85	ASP	C-N-CA	6.95	130.29	120.28
1	B	139	ASP	O-C-N	-6.95	114.75	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ALA	N-CA-CB	-6.94	99.61	110.44
1	B	120	LYS	CB-CA-C	-6.92	99.97	110.90
1	B	139	ASP	CA-C-N	6.92	135.07	121.58
1	B	139	ASP	C-N-CA	6.92	135.07	121.58
1	B	56	ILE	CB-CG1-CD1	6.91	128.32	113.80
1	A	78	THR	CA-C-O	-6.89	111.83	119.95
1	B	27	LEU	N-CA-CB	6.88	121.36	110.55
1	A	142	ALA	N-CA-CB	-6.88	100.00	110.12
1	B	151	GLN	CA-C-N	6.85	134.29	122.64
1	B	151	GLN	C-N-CA	6.85	134.29	122.64
1	A	10	LYS	CA-C-O	-6.84	113.65	120.70
1	B	13	ASP	N-CA-CB	6.82	119.96	110.07
1	B	19	ASN	CA-C-N	6.82	135.77	122.07
1	B	19	ASN	C-N-CA	6.82	135.77	122.07
1	B	189	ALA	CB-CA-C	6.81	121.71	110.81
1	A	179	ALA	CA-C-N	6.80	129.69	120.44
1	A	179	ALA	C-N-CA	6.80	129.69	120.44
1	B	20	ASP	CA-C-N	6.78	130.61	120.31
1	B	20	ASP	C-N-CA	6.78	130.61	120.31
1	B	56	ILE	CB-CA-C	6.75	120.62	111.97
1	A	243	ARG	CA-C-O	-6.75	113.48	121.11
1	B	135	VAL	CA-C-N	6.75	132.81	120.79
1	B	135	VAL	C-N-CA	6.75	132.81	120.79
1	B	134	ASN	CA-C-O	-6.75	113.90	120.92
1	B	248	GLU	CB-CG-CD	6.75	124.07	112.60
1	A	126	ARG	CD-NE-CZ	6.74	133.84	124.40
1	B	1	MET	O-C-N	-6.74	112.22	123.00
1	B	25	GLY	N-CA-C	-6.74	104.33	112.48
1	A	52	LEU	CA-C-O	-6.73	113.28	120.42
1	B	121	ASN	N-CA-C	6.73	121.77	113.50
1	B	249	ILE	CA-CB-CG2	6.69	121.88	110.50
1	B	249	ILE	N-CA-CB	6.69	123.03	111.39
1	B	222	ARG	CD-NE-CZ	-6.68	115.05	124.40
1	A	166	ARG	CA-C-O	6.67	127.64	119.97
1	A	209	TYR	CA-C-O	6.66	129.59	121.87
1	B	29	ILE	O-C-N	-6.65	115.66	123.04
1	A	249	ILE	N-CA-CB	6.64	119.83	111.46
1	B	248	GLU	CA-C-O	-6.64	113.34	121.11
1	B	235	ALA	CB-CA-C	6.63	117.55	110.65
1	A	211	ASN	CB-CA-C	6.63	123.61	110.42
1	A	112	ILE	O-C-N	6.62	129.03	121.94
1	B	252	TYR	CA-C-O	-6.61	114.05	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	HIS	CA-CB-CG	-6.58	107.22	113.80
1	A	165	GLN	CA-C-O	-6.58	113.69	120.54
1	A	3	GLN	N-CA-C	6.57	119.00	111.11
1	B	17	GLN	CA-C-O	-6.57	112.80	120.62
1	A	225	ARG	NH1-CZ-NH2	-6.56	110.77	119.30
1	B	78	THR	OG1-CB-CG2	6.55	122.40	109.30
1	A	150	PHE	CA-CB-CG	6.54	120.34	113.80
1	B	207	HIS	CA-C-O	-6.53	114.02	121.40
1	A	158	LYS	CA-C-O	-6.51	113.67	120.70
1	A	189	ALA	O-C-N	-6.51	115.22	122.12
1	B	222	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	B	113	THR	CA-C-O	-6.51	113.52	120.42
1	B	202	THR	CA-CB-OG1	-6.51	99.84	109.60
1	B	225	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	B	245	GLU	N-CA-C	6.50	120.79	112.34
1	B	126	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	B	62	PHE	N-CA-CB	6.49	119.42	110.01
1	A	128	ILE	CA-C-O	-6.49	112.67	120.78
1	A	24	THR	N-CA-C	6.48	119.66	111.69
1	A	33	GLN	OE1-CD-NE2	6.48	129.08	122.60
1	B	2	LYS	N-CA-C	6.48	118.88	111.11
1	A	44	LEU	CB-CA-C	6.48	120.81	110.19
1	B	202	THR	CA-CB-CG2	6.47	121.50	110.50
1	A	19	ASN	CA-C-O	-6.47	113.60	121.36
1	B	3	GLN	N-CA-C	-6.47	104.31	111.36
1	A	169	ASP	CB-CA-C	6.45	121.95	111.05
1	A	123	PRO	CB-CA-C	6.43	120.98	111.85
1	B	52	LEU	CB-CA-C	6.43	123.75	110.31
1	B	210	SER	CA-CB-OG	-6.42	98.26	111.10
1	B	169	ASP	N-CA-C	-6.42	98.08	108.41
1	B	264	ILE	N-CA-CB	6.41	122.40	111.50
1	B	223	GLU	CB-CG-CD	6.41	123.50	112.60
1	B	205	ASP	CA-CB-CG	-6.40	106.20	112.60
1	B	21	ARG	CD-NE-CZ	6.39	133.35	124.40
1	A	215	GLN	CG-CD-NE2	6.39	125.98	116.40
1	B	261	PRO	CA-C-O	-6.39	113.88	121.67
1	A	115	VAL	CA-C-O	6.38	127.61	120.85
1	B	13	ASP	O-C-N	6.38	128.98	122.09
1	B	127	ARG	CA-C-O	-6.37	112.81	120.65
1	A	29	ILE	N-CA-C	-6.37	99.50	108.80
1	A	195	GLU	CB-CA-C	-6.36	98.70	109.83
1	A	99	ARG	NE-CZ-NH2	6.35	124.91	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	THR	CA-C-O	-6.34	113.51	120.36
1	A	57	HIS	CA-C-O	-6.34	113.83	120.55
1	B	2	LYS	CG-CD-CE	6.32	125.83	111.30
1	A	69	ILE	N-CA-C	6.31	120.87	112.98
1	A	11	VAL	CB-CA-C	6.31	120.66	112.14
1	A	243	ARG	NH1-CZ-NH2	6.31	127.50	119.30
1	B	85	ASP	CB-CG-OD1	-6.30	103.90	118.40
1	A	62	PHE	CA-CB-CG	6.30	120.10	113.80
1	B	29	ILE	CB-CA-C	6.28	120.09	110.55
1	B	176	PHE	CA-CB-CG	6.26	120.06	113.80
1	B	181	TYR	CA-C-O	-6.26	113.91	120.55
1	B	78	THR	CA-CB-CG2	6.25	121.13	110.50
1	B	139	ASP	CA-C-O	6.25	127.38	120.63
1	A	60	LEU	CB-CA-C	6.24	121.15	110.79
1	A	253	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	13	ASP	CA-C-O	-6.21	114.30	120.70
1	A	56	ILE	N-CA-CB	6.21	118.52	110.57
1	B	217	HIS	CA-C-O	6.21	127.54	120.90
1	A	235	ALA	O-C-N	6.21	127.44	120.68
1	A	218	LEU	CB-CA-C	6.21	120.62	110.88
1	A	130	VAL	O-C-N	-6.19	116.52	123.20
1	A	49	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	A	244	PHE	CA-CB-CG	-6.18	107.62	113.80
1	B	157	GLY	CA-C-O	-6.17	112.09	119.00
1	B	108	HIS	N-CA-CB	6.17	122.16	111.00
1	B	255	HIS	N-CA-C	-6.16	101.08	110.07
1	A	241	ASP	N-CA-C	6.15	120.92	113.17
1	A	129	ILE	CA-C-O	-6.15	114.15	121.28
1	A	138	LEU	CA-C-N	6.14	130.43	120.60
1	A	138	LEU	C-N-CA	6.14	130.43	120.60
1	A	96	LYS	CB-CG-CD	6.14	125.42	111.30
1	A	75	ASN	CB-CG-ND2	-6.14	107.19	116.40
1	A	76	ASN	OD1-CG-ND2	6.13	128.73	122.60
1	A	237	GLU	CB-CG-CD	6.12	123.01	112.60
1	B	168	CYS	N-CA-CB	-6.12	100.22	110.80
1	A	28	SER	N-CA-CB	-6.11	101.07	111.69
1	A	121	ASN	CA-C-O	-6.10	112.43	119.14
1	B	101	TRP	O-C-N	6.09	126.84	121.18
1	B	85	ASP	OD1-CG-OD2	6.08	137.50	122.90
1	B	55	ILE	CA-C-O	-6.08	114.41	120.85
1	A	39	GLN	N-CA-C	-6.06	105.38	112.89
1	A	73	HIS	CA-CB-CG	-6.05	107.75	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LEU	N-CA-CB	-6.04	100.47	110.02
1	A	93	VAL	CB-CA-C	6.04	121.19	111.29
1	A	39	GLN	CB-CA-C	6.04	122.60	109.99
1	B	162	GLN	CA-C-O	-6.03	113.85	120.36
1	B	156	ASP	O-C-N	6.02	130.12	122.65
1	A	76	ASN	CA-CB-CG	-6.01	106.59	112.60
1	A	99	ARG	CB-CG-CD	6.01	125.12	111.30
1	A	192	CYS	CA-C-O	-6.00	112.17	119.43
1	B	43	PRO	CB-CA-C	6.00	121.25	113.09
1	B	241	ASP	CA-C-O	-6.00	113.73	121.17
1	B	126	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	133	TRP	N-CA-C	5.96	118.87	109.39
1	B	206	THR	CA-C-O	-5.96	114.34	120.54
1	B	99	ARG	CD-NE-CZ	-5.95	116.07	124.40
1	A	209	TYR	CA-C-N	5.95	128.25	120.28
1	A	209	TYR	C-N-CA	5.95	128.25	120.28
1	B	138	LEU	CA-C-N	5.94	128.52	120.38
1	B	138	LEU	C-N-CA	5.94	128.52	120.38
1	B	74	GLU	CB-CA-C	-5.94	97.80	110.32
1	A	149	PHE	CA-CB-CG	5.93	119.73	113.80
1	B	53	ARG	CA-C-O	5.92	126.70	120.42
1	A	19	ASN	CB-CG-OD1	-5.91	108.98	120.80
1	B	157	GLY	N-CA-C	-5.91	107.73	115.47
1	B	263	ALA	CB-CA-C	-5.91	100.36	110.22
1	B	97	GLN	CA-CB-CG	5.90	125.91	114.10
1	A	18	LYS	CA-CB-CG	5.90	125.90	114.10
1	A	115	VAL	N-CA-CB	-5.90	101.73	110.58
1	A	166	ARG	CA-C-N	5.90	131.12	122.39
1	A	166	ARG	C-N-CA	5.90	131.12	122.39
1	A	113	THR	CA-C-O	-5.89	112.13	119.38
1	B	104	PRO	N-CA-C	-5.89	105.99	114.18
1	B	118	GLN	CA-C-N	5.86	128.14	120.28
1	B	118	GLN	C-N-CA	5.86	128.14	120.28
1	A	166	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	B	237	GLU	CA-CB-CG	5.85	125.80	114.10
1	B	258	ILE	CA-C-N	5.85	131.07	123.00
1	B	258	ILE	C-N-CA	5.85	131.07	123.00
1	B	3	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	B	139	ASP	N-CA-CB	-5.84	101.31	110.06
1	A	225	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	41	GLY	N-CA-C	-5.83	104.03	110.96
1	B	24	THR	N-CA-CB	5.81	119.05	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	A	19	ASN	CA-C-N	-5.80	113.07	122.82
1	A	19	ASN	C-N-CA	-5.80	113.07	122.82
1	A	2	LYS	CA-C-N	5.79	128.35	120.54
1	A	2	LYS	C-N-CA	5.79	128.35	120.54
1	A	5	LEU	CA-C-O	-5.78	114.43	120.55
1	B	185	VAL	CB-CA-C	5.77	119.27	111.88
1	B	56	ILE	CA-CB-CG1	5.77	120.20	110.40
1	B	213	MET	N-CA-CB	5.76	118.79	110.20
1	B	94	TYR	CB-CG-CD2	-5.76	112.16	120.80
1	B	98	TRP	N-CA-CB	5.76	118.36	110.01
1	B	175	PRO	CA-C-N	5.76	128.46	120.63
1	B	175	PRO	C-N-CA	5.76	128.46	120.63
1	A	203	GLY	N-CA-C	5.76	122.00	111.12
1	A	115	VAL	O-C-N	-5.75	115.90	121.83
1	B	135	VAL	O-C-N	-5.75	116.09	121.90
1	A	54	SER	CA-CB-OG	-5.75	99.60	111.10
1	B	151	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	222	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	B	129	ILE	CA-C-N	5.73	131.12	122.98
1	B	129	ILE	C-N-CA	5.73	131.12	122.98
1	B	176	PHE	CA-C-N	5.73	127.95	120.28
1	B	176	PHE	C-N-CA	5.73	127.95	120.28
1	A	187	MET	CB-CA-C	5.72	119.94	110.90
1	B	155	ALA	N-CA-CB	5.72	120.16	110.49
1	A	70	ALA	CB-CA-C	5.72	119.86	110.88
1	A	122	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	104	PRO	CA-C-O	-5.71	111.27	118.86
1	B	120	LYS	CA-C-O	-5.69	114.84	120.70
1	B	29	ILE	CA-C-N	5.69	131.02	123.00
1	B	29	ILE	C-N-CA	5.69	131.02	123.00
1	B	33	GLN	CB-CG-CD	5.69	122.27	112.60
1	B	26	THR	OG1-CB-CG2	5.69	120.67	109.30
1	A	219	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	B	154	VAL	CA-C-O	5.66	126.33	120.39
1	A	70	ALA	N-CA-CB	-5.66	101.81	110.01
1	A	212	HIS	N-CA-CB	5.65	119.08	110.95
1	B	153	TYR	CA-C-O	-5.64	112.60	120.21
1	A	40	ASP	CA-C-O	-5.64	112.32	119.31
1	A	59	LEU	CB-CA-C	-5.64	101.27	110.85
1	A	64	GLN	CB-CG-CD	-5.63	103.02	112.60
1	B	16	THR	CA-CB-OG1	-5.63	101.15	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	THR	OG1-CB-CG2	5.63	120.56	109.30
1	A	119	LEU	O-C-N	5.62	128.08	122.12
1	B	113	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	72	LEU	CA-C-O	-5.62	114.92	120.82
1	B	73	HIS	CA-CB-CG	-5.61	108.19	113.80
1	B	257	GLY	O-C-N	-5.59	115.43	122.70
1	A	16	THR	CA-CB-OG1	-5.58	101.23	109.60
1	B	151	GLN	CA-C-O	5.58	127.29	120.60
1	A	105	ASP	CB-CA-C	5.57	119.70	111.17
1	A	156	ASP	O-C-N	5.57	130.00	122.59
1	A	21	ARG	CG-CD-NE	-5.56	99.76	112.00
1	B	27	LEU	N-CA-C	-5.56	99.45	108.52
1	A	135	VAL	CA-C-N	5.55	130.67	120.79
1	A	135	VAL	C-N-CA	5.55	130.67	120.79
1	B	54	SER	CA-C-O	-5.55	113.25	119.79
1	A	30	PHE	CA-CB-CG	5.54	119.34	113.80
1	B	153	TYR	N-CA-CB	-5.54	101.51	110.71
1	B	94	TYR	N-CA-C	5.54	120.45	111.37
1	A	219	GLN	CA-C-O	5.53	126.63	120.82
1	A	193	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	39	GLN	CA-CB-CG	-5.53	103.05	114.10
1	A	151	GLN	CG-CD-NE2	5.52	124.68	116.40
1	B	94	TYR	CB-CG-CD1	5.52	129.08	120.80
1	A	195	GLU	OE1-CD-OE2	5.51	136.13	122.90
1	A	264	ILE	N-CA-C	5.51	126.43	111.00
1	B	107	ARG	CA-C-O	5.51	128.38	120.51
1	A	99	ARG	NH1-CZ-NH2	-5.50	112.14	119.30
1	B	165	GLN	CB-CA-C	5.50	119.75	110.79
1	B	14	GLU	CA-C-O	-5.49	112.78	119.32
1	B	95	GLY	CA-C-N	5.49	127.57	120.44
1	B	95	GLY	C-N-CA	5.49	127.57	120.44
1	A	9	GLN	O-C-N	-5.49	116.30	122.12
1	A	34	MET	CB-CG-SD	-5.47	96.28	112.70
1	A	106	GLY	N-CA-C	5.47	123.50	115.08
1	A	48	LYS	O-C-N	5.47	129.51	123.33
1	A	123	PRO	CA-C-O	5.47	127.00	119.18
1	A	237	GLU	CG-CD-OE1	5.45	130.94	118.40
1	B	104	PRO	CB-CA-C	5.45	120.08	111.31
1	B	80	TRP	O-C-N	5.45	129.41	122.39
1	A	210	SER	N-CA-CB	-5.44	102.12	110.12
1	B	208	LEU	CB-CG-CD1	5.44	127.02	110.70
1	A	95	GLY	CA-C-N	5.43	127.50	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLY	C-N-CA	5.43	127.50	120.44
1	B	99	ARG	N-CA-C	5.43	120.02	112.90
1	A	163	LEU	CA-C-O	-5.43	115.02	121.16
1	B	126	ARG	N-CA-C	-5.43	106.24	112.92
1	A	126	ARG	CB-CG-CD	5.43	123.79	111.30
1	B	133	TRP	O-C-N	5.43	129.50	122.71
1	B	33	GLN	CG-CD-OE1	5.42	131.65	120.80
1	A	189	ALA	CA-C-N	5.42	127.99	120.29
1	A	189	ALA	C-N-CA	5.42	127.99	120.29
1	A	107	ARG	CA-CB-CG	-5.42	103.26	114.10
1	B	250	GLU	CA-CB-CG	5.42	124.94	114.10
1	B	250	GLU	N-CA-CB	5.42	121.23	111.37
1	A	166	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	87	ASN	CB-CG-OD1	-5.40	109.99	120.80
1	B	145	PRO	CA-C-N	5.40	129.63	120.88
1	B	145	PRO	C-N-CA	5.40	129.63	120.88
1	B	92	PRO	N-CA-CB	5.40	106.03	102.25
1	B	81	ASP	N-CA-C	5.40	117.16	111.28
1	A	17	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	A	114	THR	CA-CB-CG2	5.38	119.64	110.50
1	B	22	THR	N-CA-C	-5.38	106.22	112.89
1	B	245	GLU	CA-C-N	5.37	129.69	120.72
1	B	245	GLU	C-N-CA	5.37	129.69	120.72
1	A	190	GLN	CA-C-O	-5.37	114.73	120.42
1	A	16	THR	CB-CA-C	5.37	119.97	109.35
1	B	124	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	21	ARG	N-CA-CB	5.36	118.59	110.28
1	A	99	ARG	CA-C-O	-5.36	113.25	119.14
1	A	165	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	101	TRP	CA-C-O	-5.35	114.19	119.49
1	B	42	PHE	O-C-N	5.34	126.15	121.18
1	B	169	ASP	CB-CA-C	5.34	119.63	110.81
1	B	259	LYS	N-CA-CB	-5.34	102.18	110.57
1	B	28	SER	N-CA-C	5.33	117.93	109.50
1	A	255	HIS	N-CA-C	-5.33	101.23	109.87
1	B	183	LEU	O-C-N	5.32	127.84	122.09
1	A	68	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	3	GLN	CB-CA-C	-5.31	102.32	110.81
1	A	260	ALA	CA-C-O	-5.31	114.50	119.91
1	B	206	THR	CB-CA-C	5.31	119.27	110.78
1	A	178	ILE	CB-CA-C	5.30	119.54	112.22
1	A	165	GLN	CG-CD-NE2	5.30	124.35	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ARG	CA-CB-CG	5.29	124.69	114.10
1	A	132	ALA	CA-C-O	5.29	125.18	119.15
1	A	71	TYR	O-C-N	5.29	127.59	122.09
1	A	55	ILE	N-CA-C	-5.28	105.57	110.53
1	A	16	THR	CA-CB-CG2	5.27	119.46	110.50
1	A	225	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	A	33	GLN	CG-CD-OE1	-5.24	110.31	120.80
1	A	89	ASP	O-C-N	5.24	128.93	123.06
1	B	69	ILE	CA-CB-CG1	5.24	119.31	110.40
1	A	199	PHE	N-CA-CB	5.23	118.77	110.55
1	B	199	PHE	N-CA-C	-5.23	98.73	107.99
1	B	2	LYS	CB-CA-C	-5.23	102.44	110.81
1	B	169	ASP	CA-C-O	-5.23	114.99	120.58
1	B	30	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	88	GLY	N-CA-C	-5.22	107.60	115.32
1	B	14	GLU	N-CA-C	5.21	120.28	113.30
1	B	57	HIS	CA-C-O	-5.20	115.04	120.55
1	A	210	SER	CA-C-O	5.19	126.06	120.55
1	A	151	GLN	N-CA-CB	-5.19	101.60	111.00
1	B	96	LYS	CA-C-N	5.19	127.66	120.29
1	B	96	LYS	C-N-CA	5.19	127.66	120.29
1	A	119	LEU	CB-CA-C	5.19	119.40	110.79
1	A	4	TYR	CB-CG-CD1	5.18	128.56	120.80
1	A	86	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	62	PHE	CA-C-O	-5.17	115.39	120.82
1	B	163	LEU	CA-C-N	5.17	130.45	123.11
1	B	163	LEU	C-N-CA	5.17	130.45	123.11
1	B	105	ASP	N-CA-C	5.17	119.08	112.26
1	A	182	ALA	CA-C-N	5.16	127.45	120.44
1	A	182	ALA	C-N-CA	5.16	127.45	120.44
1	B	82	GLU	O-C-N	5.15	129.57	122.46
1	A	253	ASP	O-C-N	5.15	125.55	121.17
1	B	170	VAL	N-CA-C	5.15	115.36	110.42
1	A	65	GLY	CA-C-N	5.14	128.77	121.42
1	A	65	GLY	C-N-CA	5.14	128.77	121.42
1	B	250	GLU	CB-CA-C	-5.14	98.64	109.38
1	A	183	LEU	O-C-N	5.14	127.64	122.09
1	A	230	LEU	CA-C-N	-5.14	115.85	122.99
1	A	230	LEU	C-N-CA	-5.14	115.85	122.99
1	A	48	LYS	N-CA-C	-5.12	100.94	108.99
1	A	91	GLY	N-CA-C	-5.11	101.91	112.34
1	B	101	TRP	CA-C-O	-5.11	114.43	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	LEU	CA-C-O	5.11	125.84	120.42
1	A	243	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	B	66	ASP	CB-CG-OD1	-5.11	106.65	118.40
1	A	141	MET	O-C-N	5.10	129.04	123.22
1	B	28	SER	CB-CA-C	-5.10	98.72	109.38
1	B	37	ASN	N-CA-C	-5.09	100.86	108.96
1	B	124	ASP	CA-C-N	5.09	128.07	120.90
1	B	124	ASP	C-N-CA	5.09	128.07	120.90
1	A	149	PHE	CA-C-O	-5.08	114.43	120.43
1	A	184	LEU	CA-C-O	-5.08	115.66	121.00
1	B	241	ASP	CB-CA-C	5.08	119.87	111.23
1	A	138	LEU	O-C-N	-5.08	116.74	122.12
1	A	149	PHE	CB-CA-C	5.08	119.00	109.86
1	B	24	THR	CA-CB-CG2	5.08	119.13	110.50
1	A	43	PRO	CB-CA-C	5.06	119.91	111.56
1	A	67	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	93	VAL	CA-C-N	5.05	131.19	121.54
1	A	93	VAL	C-N-CA	5.05	131.19	121.54
1	B	135	VAL	CA-C-O	5.05	126.15	120.64
1	A	32	HIS	CA-CB-CG	-5.04	108.76	113.80
1	B	115	VAL	N-CA-C	5.04	115.26	110.42
1	B	11	VAL	CA-C-N	5.04	126.98	120.44
1	B	11	VAL	C-N-CA	5.04	126.98	120.44
1	A	235	ALA	N-CA-CB	5.03	118.78	110.38
1	A	156	ASP	CA-C-O	-5.03	113.32	120.51
1	A	246	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	167	SER	N-CA-C	5.03	116.60	108.26
1	B	246	ASP	O-C-N	5.02	129.16	122.43
1	B	137	GLU	CB-CA-C	-5.01	102.64	110.85
1	B	177	ASN	CB-CG-ND2	-5.01	108.89	116.40
1	A	15	GLY	O-C-N	5.00	129.47	122.82

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	127	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	21	ARG	Sidechain
1	B	243	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	2146	0	2073	89	0
1	B	2146	0	2073	93	0
2	A	20	0	8	0	0
2	B	20	0	9	0	0
3	A	35	0	21	3	0
3	B	35	0	21	1	0
4	A	113	0	0	8	0
4	B	85	0	0	9	0
All	All	4600	0	4205	175	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 20.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:HD3	1:B:244:PHE:H	1.18	1.09
1:B:243:ARG:CD	1:B:244:PHE:H	1.68	1.07
1:A:8:MET:HE2	1:A:220:LEU:HD13	1.43	0.98
1:A:215:GLN:HE21	1:A:215:GLN:H	1.16	0.94
1:A:172:LEU:HD12	3:A:266:CB3:OE2	1.74	0.87
1:A:234:ARG:NH2	1:A:246:ASP:OD2	2.11	0.83
1:B:245:GLU:OE2	4:B:677:HOH:O	1.96	0.83
1:B:107:ARG:HG3	4:B:704:HOH:O	1.75	0.83
1:B:103:THR:HG22	1:B:109:ILE:HD11	1.61	0.82
1:A:44:LEU:CD2	1:A:52:LEU:HD21	2.09	0.81
1:A:22:THR:O	1:A:264:ILE:HD11	1.79	0.81
1:B:243:ARG:CD	1:B:244:PHE:N	2.43	0.80
1:A:202:THR:HG21	1:B:202:THR:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD22	1:B:187:MET:HE2	1.64	0.78
1:A:22:THR:O	1:A:264:ILE:CD1	2.31	0.78
1:B:22:THR:HG21	1:B:263:ALA:HB1	1.66	0.78
1:A:195:GLU:HA	4:A:570:HOH:O	1.85	0.77
1:A:37:ASN:HD22	1:A:39:GLN:H	1.31	0.75
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.17	0.75
1:B:1:MET:HE1	1:B:43:PRO:HA	1.68	0.74
1:B:66:ASP:OD2	4:B:689:HOH:O	2.05	0.73
1:B:59:LEU:HD23	1:B:187:MET:HE1	1.71	0.73
1:A:56:ILE:HG12	1:A:183:LEU:HD21	1.72	0.72
1:A:172:LEU:HD12	3:A:266:CB3:HOE2	1.52	0.72
1:A:8:MET:CE	1:A:220:LEU:HD13	2.19	0.71
1:B:243:ARG:HD2	1:B:244:PHE:H	1.55	0.71
1:B:243:ARG:HD3	1:B:244:PHE:N	1.98	0.71
1:B:77:VAL:HG23	1:B:79:ILE:HG12	1.71	0.71
1:A:37:ASN:ND2	1:A:39:GLN:H	1.90	0.70
1:B:99:ARG:NH1	1:B:110:ASP:OD1	2.25	0.70
1:A:44:LEU:HD22	1:A:52:LEU:HD21	1.72	0.69
1:B:39:GLN:HE21	1:B:158:LYS:HE3	1.56	0.69
1:B:20:ASP:OD1	1:B:22:THR:HB	1.92	0.69
1:A:15:GLY:HA3	1:A:27:LEU:HD22	1.76	0.68
1:A:105:ASP:O	4:A:602:HOH:O	2.11	0.68
1:A:172:LEU:CD1	3:A:266:CB3:OE2	2.41	0.67
1:A:37:ASN:HD21	1:A:39:GLN:HB2	1.60	0.67
1:A:87:ASN:ND2	4:A:575:HOH:O	2.28	0.67
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.78	0.66
1:A:45:VAL:HG22	1:A:50:CYS:SG	2.35	0.66
1:B:99:ARG:HH12	1:B:110:ASP:CG	2.03	0.66
1:A:22:THR:HB	1:A:264:ILE:HG12	1.78	0.64
1:A:110:ASP:OD2	1:A:113:THR:HG23	1.98	0.64
1:A:52:LEU:HD23	4:A:619:HOH:O	1.98	0.63
1:A:1:MET:HE3	1:A:227:LEU:HD21	1.80	0.63
1:B:215:GLN:HE21	1:B:215:GLN:H	1.45	0.63
1:B:2:LYS:HE2	4:B:716:HOH:O	1.99	0.62
1:A:188:MET:HE2	1:A:239:ILE:HD13	1.82	0.62
1:A:234:ARG:HH21	1:A:246:ASP:CG	2.08	0.61
1:A:215:GLN:H	1:A:215:GLN:NE2	1.93	0.61
1:A:44:LEU:HD21	1:A:52:LEU:HD21	1.83	0.61
1:B:38:LEU:HB3	1:B:196:VAL:CG2	2.31	0.60
1:B:243:ARG:HD2	1:B:244:PHE:N	2.13	0.60
1:A:120:LYS:HG3	1:A:121:ASN:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE1	1:B:43:PRO:CA	2.31	0.60
1:B:263:ALA:HB3	3:B:266:CB3:NA2	2.17	0.60
1:A:103:THR:CG2	1:A:109:ILE:HD13	2.32	0.60
1:B:75:ASN:O	1:B:76:ASN:HB2	2.00	0.60
1:B:38:LEU:HB3	1:B:196:VAL:HG21	1.84	0.60
1:B:234:ARG:O	1:B:236:PRO:HD3	2.02	0.59
1:B:114:THR:O	1:B:118:GLN:HG3	2.02	0.59
1:A:10:LYS:HE2	1:A:32:HIS:HD2	1.66	0.59
1:A:255:HIS:HB3	1:A:256:PRO:HD2	1.84	0.59
1:B:158:LYS:HA	1:B:195:GLU:HB3	1.86	0.58
1:B:216:THR:O	1:B:220:LEU:HB2	2.03	0.58
1:B:21:ARG:HG3	1:B:22:THR:N	2.18	0.57
1:A:151:GLN:NE2	1:B:164:TYR:OH	2.37	0.57
1:A:245:GLU:H	1:A:245:GLU:CD	2.14	0.56
1:B:59:LEU:CD2	1:B:187:MET:HE1	2.36	0.55
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.71	0.55
1:A:264:ILE:CG1	1:A:264:ILE:O	2.54	0.55
1:A:79:ILE:O	1:A:83:TRP:HZ3	1.90	0.55
1:A:243:ARG:HH11	1:A:243:ARG:CB	2.20	0.55
1:B:233:LYS:HE3	1:B:248:GLU:HB2	1.88	0.55
1:B:20:ASP:HB3	1:B:25:GLY:H	1.71	0.54
1:B:237:GLU:HB2	4:B:721:HOH:O	2.07	0.54
1:A:73:HIS:HE1	1:A:81:ASP:OD1	1.91	0.54
1:A:110:ASP:CG	1:A:113:THR:HG23	2.33	0.54
1:A:16:THR:HG22	4:A:597:HOH:O	2.07	0.54
1:A:44:LEU:HD11	1:A:50:CYS:HB2	1.90	0.54
1:A:73:HIS:CE1	1:A:81:ASP:OD1	2.62	0.53
1:A:1:MET:HE3	1:A:227:LEU:HD11	1.90	0.53
1:A:51:HIS:HB3	4:A:620:HOH:O	2.09	0.53
1:A:22:THR:O	1:A:264:ILE:HD13	2.08	0.53
1:A:36:PHE:CE1	1:A:178:ILE:HD13	2.43	0.53
1:A:243:ARG:HB2	1:A:243:ARG:NH1	2.24	0.53
1:B:65:GLY:CA	1:B:99:ARG:HG3	2.39	0.53
1:B:235:ALA:HB1	4:B:555:HOH:O	2.08	0.52
1:A:27:LEU:HD12	1:A:213:MET:HE1	1.90	0.52
1:A:215:GLN:HE21	1:A:215:GLN:N	1.97	0.52
1:A:43:PRO:HB2	1:A:178:ILE:HD11	1.90	0.52
1:B:18:LYS:HB2	1:B:26:THR:HG22	1.91	0.52
1:B:174:LEU:O	1:B:178:ILE:HG13	2.09	0.51
1:B:130:VAL:HG13	1:B:150:PHE:CE1	2.45	0.51
1:B:73:HIS:HE2	1:B:81:ASP:CG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:HB3	1:B:226:PRO:CD	2.41	0.51
1:B:262:VAL:HG13	1:B:264:ILE:CD1	2.40	0.51
1:B:170:VAL:HB	1:B:208:LEU:HD13	1.92	0.51
1:A:37:ASN:ND2	1:A:39:GLN:HB2	2.25	0.51
1:B:255:HIS:HB3	1:B:256:PRO:HD2	1.92	0.50
1:B:226:PRO:HD2	4:B:660:HOH:O	2.10	0.50
1:B:34:MET:HE1	1:B:174:LEU:HD21	1.94	0.50
1:B:53:ARG:HA	1:B:244:PHE:CE1	2.46	0.50
1:B:71:TYR:OH	1:B:243:ARG:NH1	2.44	0.50
1:B:229:LYS:CA	1:B:229:LYS:HZ2	2.25	0.50
1:A:135:VAL:HA	1:A:138:LEU:HD22	1.93	0.50
1:A:16:THR:HG21	1:B:155:ALA:HB1	1.94	0.49
1:A:18:LYS:HE3	1:B:154:VAL:O	2.11	0.49
1:B:39:GLN:NE2	1:B:158:LYS:HE3	2.24	0.49
1:A:11:VAL:HG22	1:A:208:LEU:HD22	1.93	0.49
1:B:46:THR:O	1:B:255:HIS:HD2	1.94	0.49
1:B:243:ARG:O	1:B:244:PHE:C	2.55	0.49
1:A:222:ARG:NH1	1:A:256:PRO:O	2.44	0.49
1:A:187:MET:HE3	1:A:242:TYR:CD2	2.47	0.48
1:A:195:GLU:HG3	4:A:565:HOH:O	2.12	0.48
1:B:69:ILE:HA	1:B:72:LEU:HD12	1.94	0.48
1:A:225:ARG:HD3	1:A:253:ASP:O	2.13	0.48
1:B:158:LYS:HG2	1:B:195:GLU:CG	2.44	0.48
1:A:65:GLY:HA2	1:A:95:GLY:O	2.12	0.48
1:B:10:LYS:HG3	1:B:14:GLU:OE2	2.13	0.48
1:B:58:GLU:O	1:B:61:TRP:HB3	2.14	0.48
1:B:56:ILE:HD11	1:B:244:PHE:HA	1.96	0.47
1:B:10:LYS:NZ	1:B:32:HIS:HD2	2.12	0.47
1:B:53:ARG:HB2	1:B:53:ARG:NH1	2.29	0.47
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.78	0.47
1:B:183:LEU:HD22	1:B:187:MET:CE	2.39	0.46
1:B:233:LYS:HE3	1:B:248:GLU:CB	2.45	0.46
1:A:202:THR:HG21	1:B:202:THR:CG2	2.41	0.46
1:B:68:ASN:ND2	1:B:89:ASP:OD2	2.46	0.46
1:A:135:VAL:HB	1:B:101:TRP:CE2	2.51	0.45
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.68	0.45
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.51	0.45
1:A:69:ILE:HD13	1:A:84:ALA:CB	2.46	0.45
1:A:103:THR:HG22	1:B:136:GLY:HA2	1.99	0.45
1:A:174:LEU:O	1:A:178:ILE:HG23	2.16	0.45
1:A:134:ASN:C	1:A:134:ASN:HD22	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:CB	1:A:243:ARG:NH1	2.80	0.44
1:B:53:ARG:HA	1:B:244:PHE:HE1	1.81	0.44
1:B:61:TRP:HH2	1:B:90:LEU:CD1	2.30	0.44
1:B:147:HIS:HB2	1:B:163:LEU:HD21	1.99	0.44
1:B:158:LYS:HG2	1:B:195:GLU:HB3	2.00	0.44
1:B:215:GLN:H	1:B:215:GLN:NE2	2.14	0.44
1:A:26:THR:HB	1:A:207:HIS:HB2	2.00	0.44
1:A:153:TYR:CE2	1:A:155:ALA:HB2	2.53	0.43
1:A:37:ASN:HD22	1:A:37:ASN:C	2.27	0.43
1:B:56:ILE:C	1:B:56:ILE:HD13	2.44	0.43
1:A:22:THR:CB	1:A:264:ILE:HG12	2.45	0.43
1:A:234:ARG:HD3	1:A:246:ASP:OD1	2.19	0.43
1:B:225:ARG:HD2	1:B:253:ASP:O	2.19	0.43
1:B:170:VAL:HG23	1:B:207:HIS:O	2.19	0.42
1:A:79:ILE:HG13	1:A:80:TRP:CD1	2.54	0.42
1:B:67:THR:HG21	1:B:96:LYS:HB2	2.01	0.42
1:A:187:MET:HE3	1:A:242:TYR:CG	2.54	0.42
1:B:71:TYR:HB3	4:B:689:HOH:O	2.20	0.42
1:A:27:LEU:HD11	4:A:603:HOH:O	2.19	0.42
1:B:52:LEU:HD13	1:B:249:ILE:HG12	2.01	0.42
1:B:73:HIS:NE2	1:B:81:ASP:OD1	2.43	0.42
1:B:129:ILE:HG21	1:B:149:PHE:CZ	2.54	0.42
1:B:225:ARG:CB	1:B:226:PRO:CD	2.97	0.42
1:A:55:ILE:HD13	1:A:179:ALA:HB3	2.02	0.41
1:A:147:HIS:HB2	1:A:163:LEU:HD11	2.02	0.41
1:A:49:ARG:HH11	1:A:49:ARG:HD2	1.41	0.41
1:A:86:GLU:H	1:A:86:GLU:CD	2.28	0.41
1:B:18:LYS:O	1:B:25:GLY:HA2	2.21	0.41
1:A:119:LEU:O	1:A:123:PRO:HB3	2.20	0.41
1:B:262:VAL:HG13	1:B:264:ILE:HD11	2.03	0.41
1:B:215:GLN:HG2	1:B:258:ILE:HG22	2.02	0.41
1:A:181:TYR:O	1:A:185:VAL:HG23	2.20	0.40
1:B:230:LEU:HD23	1:B:249:ILE:HG23	2.03	0.40
1:A:48:LYS:HG2	1:A:219:GLN:NE2	2.36	0.40
1:B:259:LYS:HE2	1:B:259:LYS:HB3	1.83	0.40
1:B:17:GLN:HG2	4:B:713:HOH:O	2.20	0.40
1:B:126:ARG:HH21	1:B:126:ARG:HD3	1.78	0.40
1:A:110:ASP:OD2	1:A:113:THR:CG2	2.66	0.40
1:B:213:MET:O	1:B:217:HIS:CD2	2.74	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	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	30	20
1	B	262/264 (99%)	239 (91%)	18 (7%)	5 (2%)	6	1
All	All	524/528 (99%)	488 (93%)	30 (6%)	6 (1%)	11	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	ILE
1	B	257	GLY
1	B	107	ARG
1	B	205	ASP
1	B	93	VAL
1	A	93	VAL

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	232/232 (100%)	205 (88%)	27 (12%)	5	1
1	B	232/232 (100%)	194 (84%)	38 (16%)	2	0
All	All	464/464 (100%)	399 (86%)	65 (14%)	3	1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	VAL
1	A	16	THR
1	A	27	LEU
1	A	28	SER
1	A	37	ASN
1	A	48	LYS
1	A	59	LEU
1	A	60	LEU
1	A	86	GLU
1	A	109	ILE
1	A	113	THR
1	A	115	VAL
1	A	125	SER
1	A	178	ILE
1	A	208	LEU
1	A	210	SER
1	A	215	GLN
1	A	220	LEU
1	A	223	GLU
1	A	225	ARG
1	A	230	LEU
1	A	245	GLU
1	A	249	ILE
1	A	259	LYS
1	A	262	VAL
1	A	264	ILE
1	B	1	MET
1	B	2	LYS
1	B	5	LEU
1	B	8	MET
1	B	26	THR
1	B	38	LEU
1	B	47	THR
1	B	48	LYS
1	B	50	CYS
1	B	52	LEU
1	B	53	ARG
1	B	56	ILE
1	B	66	ASP
1	B	69	ILE
1	B	77	VAL
1	B	78	THR

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Mol	Chain	Res	Type
1	B	82	GLU
1	B	96	LYS
1	B	116	LEU
1	B	120	LYS
1	B	130	VAL
1	B	163	LEU
1	B	183	LEU
1	B	208	LEU
1	B	215	GLN
1	B	227	LEU
1	B	229	LYS
1	B	231	ILE
1	B	234	ARG
1	B	241	ASP
1	B	243	ARG
1	B	245	GLU
1	B	249	ILE
1	B	250	GLU
1	B	253	ASP
1	B	258	ILE
1	B	259	LYS
1	B	264	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	32	HIS
1	A	33	GLN
1	A	37	ASN
1	A	73	HIS
1	A	75	ASN
1	A	87	ASN
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	191	GLN
1	A	215	GLN
1	A	219	GLN

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Mol	Chain	Res	Type
1	B	32	HIS
1	B	51	HIS
1	B	75	ASN
1	B	76	ASN
1	B	117	ASN
1	B	121	ASN
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	$\# Z > 2$
3	CB3	B	266	-	37,37,37	3.07	17 (45%)	50,51,51	3.04	21 (42%)
2	UMP	B	265	1	21,21,21	2.60	7 (33%)	30,31,31	3.81	13 (43%)
3	CB3	A	266	-	37,37,37	3.20	15 (40%)	50,51,51	3.61	19 (38%)
2	UMP	A	265	1	21,21,21	2.72	8 (38%)	30,31,31	2.73	10 (33%)

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	CB3	B	266	-	-	8/27/28/28	0/3/3/3
2	UMP	B	265	1	-	1/10/22/22	0/2/2/2
3	CB3	A	266	-	-	9/27/28/28	0/3/3/3
2	UMP	A	265	1	-	1/10/22/22	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	266	CB3	C4A-C4	-8.50	1.33	1.48
3	B	266	CB3	C4A-C4	-8.50	1.33	1.48
3	A	266	CB3	CG-CD	8.48	1.70	1.50
2	B	265	UMP	C1'-N1	-6.97	1.30	1.48
2	A	265	UMP	C1'-N1	-6.86	1.30	1.48
3	B	266	CB3	CG-CD	6.79	1.66	1.50
3	A	266	CB3	C2-NA2	5.97	1.48	1.34
3	A	266	CB3	CP1-CP2	5.72	1.55	1.46
3	B	266	CB3	CP1-CP2	5.71	1.55	1.46
3	B	266	CB3	C2-NA2	5.50	1.47	1.34
3	B	266	CB3	CP1-N10	5.33	1.51	1.46
2	B	265	UMP	C2-N1	5.25	1.46	1.38
3	A	266	CB3	OE1-CD	5.13	1.38	1.22
3	B	266	CB3	C9-N10	4.41	1.52	1.46
2	A	265	UMP	C6-C5	4.37	1.45	1.35
3	B	266	CB3	O1-CT	4.19	1.34	1.22
2	A	265	UMP	C2'-C1'	4.18	1.63	1.52
3	A	266	CB3	C4-N3	-4.14	1.30	1.38
3	A	266	CB3	C7-C6	4.09	1.47	1.38
2	A	265	UMP	O2-C2	-4.07	1.15	1.23
3	A	266	CB3	C9-N10	3.97	1.52	1.46
2	B	265	UMP	C2'-C1'	3.90	1.62	1.52
3	B	266	CB3	C4-N3	-3.88	1.30	1.38
3	A	266	CB3	C8-C7	-3.74	1.32	1.38
2	B	265	UMP	C6-C5	3.53	1.43	1.35
2	A	265	UMP	O5'-C5'	-3.52	1.31	1.44
2	A	265	UMP	C5'-C4'	-3.46	1.41	1.51
3	A	266	CB3	OE2-CD	3.40	1.42	1.30
2	B	265	UMP	O2-C2	-3.36	1.17	1.23
2	A	265	UMP	O4'-C1'	3.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	266	CB3	C14-N10	3.13	1.47	1.38
3	A	266	CB3	C2-N1	-3.02	1.30	1.37
3	B	266	CB3	C2-N1	-2.99	1.30	1.37
2	B	265	UMP	O5'-C5'	-2.81	1.33	1.44
3	B	266	CB3	OE1-CD	2.76	1.31	1.22
3	B	266	CB3	C16-C15	2.71	1.43	1.38
3	A	266	CB3	C11-C	2.68	1.56	1.50
3	A	266	CB3	C8A-N1	-2.66	1.35	1.39
3	B	266	CB3	C7-C6	2.65	1.44	1.38
3	B	266	CB3	C11-C	2.64	1.56	1.50
3	A	266	CB3	O1-CT	2.53	1.29	1.22
3	B	266	CB3	C8-C7	-2.45	1.34	1.38
2	B	265	UMP	O4'-C1'	2.30	1.47	1.42
3	B	266	CB3	CB-CA	2.16	1.58	1.53
2	A	265	UMP	C2-N1	2.12	1.41	1.38
3	B	266	CB3	C14-N10	2.06	1.44	1.38
3	B	266	CB3	C9-C6	-2.02	1.47	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	CB3	CA-N-C	11.84	149.96	121.56
3	A	266	CB3	OE2-CD-OE1	10.45	150.22	123.33
3	A	266	CB3	OE1-CD-CG	-8.96	94.67	123.09
3	B	266	CB3	CA-N-C	8.77	142.61	121.56
2	B	265	UMP	O2-C2-N3	-8.36	106.07	121.49
2	B	265	UMP	O4'-C1'-N1	8.35	122.69	107.86
2	A	265	UMP	C6-N1-C2	-7.79	111.52	121.00
2	B	265	UMP	C5-C6-N1	-7.67	109.37	121.84
2	A	265	UMP	C5-C6-N1	-7.62	109.45	121.84
3	A	266	CB3	CP2-CP1-N10	-7.36	106.66	113.45
2	B	265	UMP	C6-N1-C2	-7.15	112.30	121.00
2	B	265	UMP	C4-N3-C2	-6.80	118.17	126.61
3	B	266	CB3	CP2-CP1-N10	-6.70	107.27	113.45
3	B	266	CB3	C9-C6-C7	-6.43	108.91	120.75
3	B	266	CB3	O-C-N	-5.86	111.32	122.47
3	A	266	CB3	CB-CA-N	5.69	122.17	110.91
3	B	266	CB3	CG-CB-CA	-5.68	102.69	113.16
3	A	266	CB3	O2-CT-O1	5.62	136.82	124.08
2	B	265	UMP	C2'-C1'-N1	5.59	127.79	113.81
3	B	266	CB3	CP1-N10-C9	-5.40	111.75	117.19
3	A	266	CB3	CB-CG-CD	-5.21	98.59	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	265	UMP	O4-C4-N3	5.18	126.78	119.27
3	B	266	CB3	C9-C6-C5	4.93	129.57	120.27
3	B	266	CB3	CB-CG-CD	-4.89	99.45	112.49
3	A	266	CB3	O-C-N	-4.67	113.58	122.47
3	A	266	CB3	C6-C9-N10	4.61	121.59	114.13
3	A	266	CB3	CG-CB-CA	-4.41	105.03	113.16
2	A	265	UMP	O4'-C1'-N1	4.39	115.66	107.86
3	B	266	CB3	C11-C-N	4.38	125.16	117.04
2	B	265	UMP	C6-C5-C4	-4.30	114.04	119.53
2	B	265	UMP	C1'-N1-C2	4.00	125.48	117.66
2	A	265	UMP	C2'-C1'-N1	3.98	123.76	113.81
3	A	266	CB3	O-C-C11	3.98	128.78	120.90
3	B	266	CB3	OE1-CD-CG	-3.89	110.76	123.09
3	A	266	CB3	C16-C11-C12	3.72	123.30	118.57
3	B	266	CB3	C9-N10-C14	3.70	127.14	120.72
2	A	265	UMP	C1'-N1-C2	3.61	124.73	117.66
3	A	266	CB3	C15-C16-C11	-3.56	116.99	120.80
3	B	266	CB3	CP1-N10-C14	-3.45	112.55	119.03
2	A	265	UMP	O2-C2-N3	-3.39	115.23	121.49
2	A	265	UMP	N3-C2-N1	3.39	119.30	114.89
3	B	266	CB3	OE2-CD-OE1	3.34	131.93	123.33
3	B	266	CB3	C5-C4A-C8A	3.28	122.04	119.09
3	B	266	CB3	C13-C12-C11	-3.28	117.30	120.80
3	A	266	CB3	C5-C4A-C8A	3.07	121.85	119.09
3	B	266	CB3	C15-C14-N10	-2.94	117.31	121.39
3	B	266	CB3	C4A-C5-C6	-2.80	117.03	121.38
2	B	265	UMP	N3-C2-N1	2.72	118.44	114.89
3	B	266	CB3	C6-C9-N10	2.65	118.43	114.13
2	B	265	UMP	O4'-C1'-C2'	-2.62	101.35	106.25
3	A	266	CB3	C4A-C5-C6	-2.51	117.49	121.38
3	A	266	CB3	C9-N10-C14	-2.48	116.43	120.72
2	A	265	UMP	C6-C5-C4	-2.47	116.37	119.53
2	A	265	UMP	O5'-C5'-C4'	2.44	117.30	108.99
2	B	265	UMP	O2-C2-N1	2.34	125.85	122.80
3	A	266	CB3	O1-CT-CA	-2.33	114.75	122.26
2	B	265	UMP	O4-C4-C5	-2.30	121.20	125.16
3	A	266	CB3	C9-C6-C7	-2.23	116.65	120.75
3	B	266	CB3	C16-C11-C12	2.20	121.37	118.57
3	B	266	CB3	C12-C13-C14	2.20	123.08	120.30
3	A	266	CB3	N1-C2-N3	-2.15	119.38	123.32
2	A	265	UMP	C5-C4-N3	-2.11	111.83	114.80
3	B	266	CB3	C7-C6-C5	2.09	121.43	118.55

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	266	CB3	N-CA-CB-CG
3	B	266	CB3	C6-C9-N10-C14
3	A	266	CB3	CT-CA-CB-CG
3	B	266	CB3	CT-CA-CB-CG
3	A	266	CB3	N-CA-CB-CG
3	B	266	CB3	C13-C14-N10-C9
3	B	266	CB3	C15-C14-N10-C9
3	A	266	CB3	C6-C9-N10-C14
3	A	266	CB3	N-CA-CT-O1
3	A	266	CB3	N-CA-CT-O2
2	A	265	UMP	C2'-C1'-N1-C2
3	B	266	CB3	N-CA-CT-O1
3	B	266	CB3	OE2-CD-CG-CB
3	A	266	CB3	C15-C14-N10-C9
3	B	266	CB3	OE1-CD-CG-CB
2	B	265	UMP	O4'-C4'-C5'-O5'
3	A	266	CB3	OE2-CD-CG-CB
3	A	266	CB3	OE1-CD-CG-CB
3	A	266	CB3	CT-CA-N-C

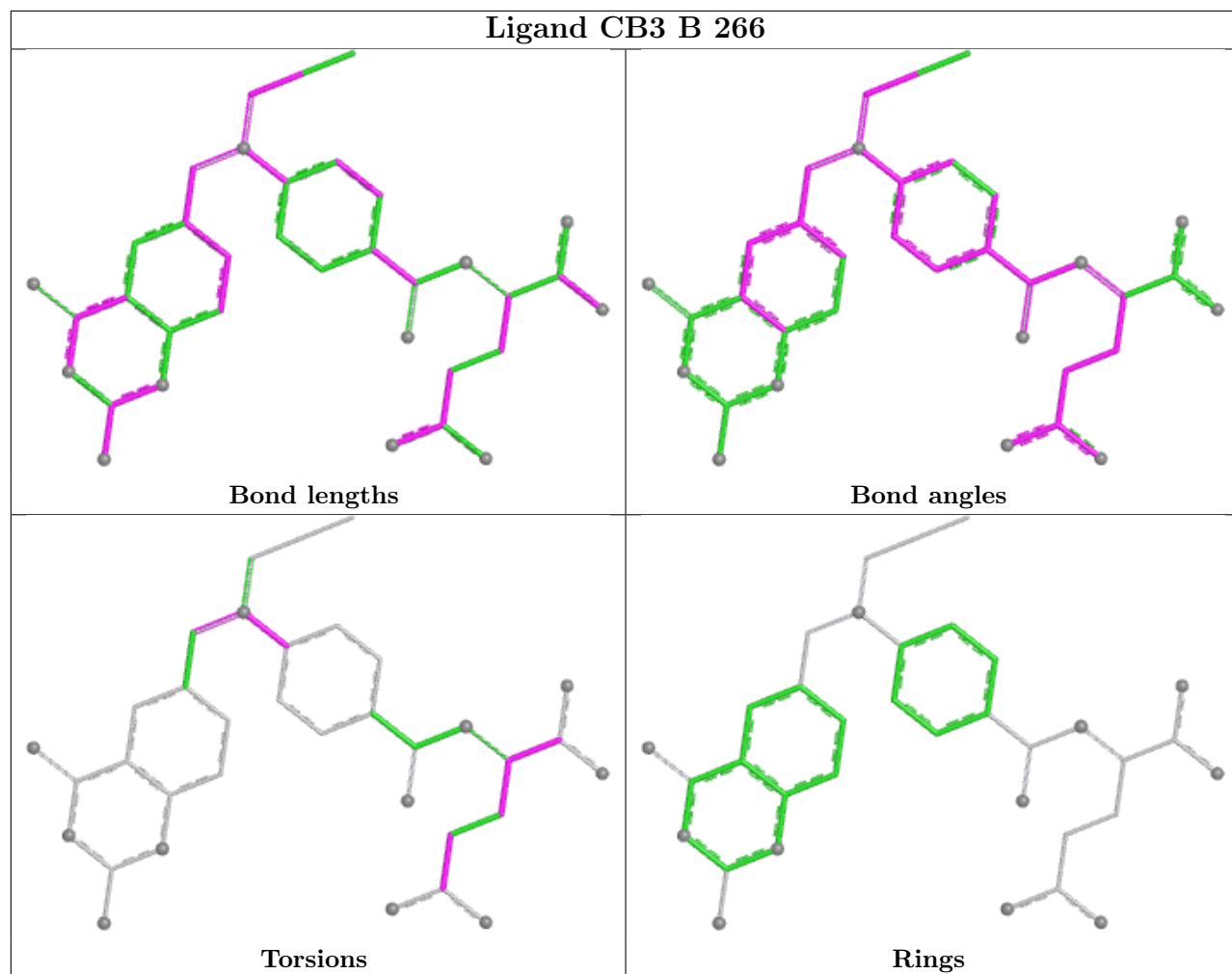
There are no ring outliers.

2 monomers are involved in 4 short contacts:

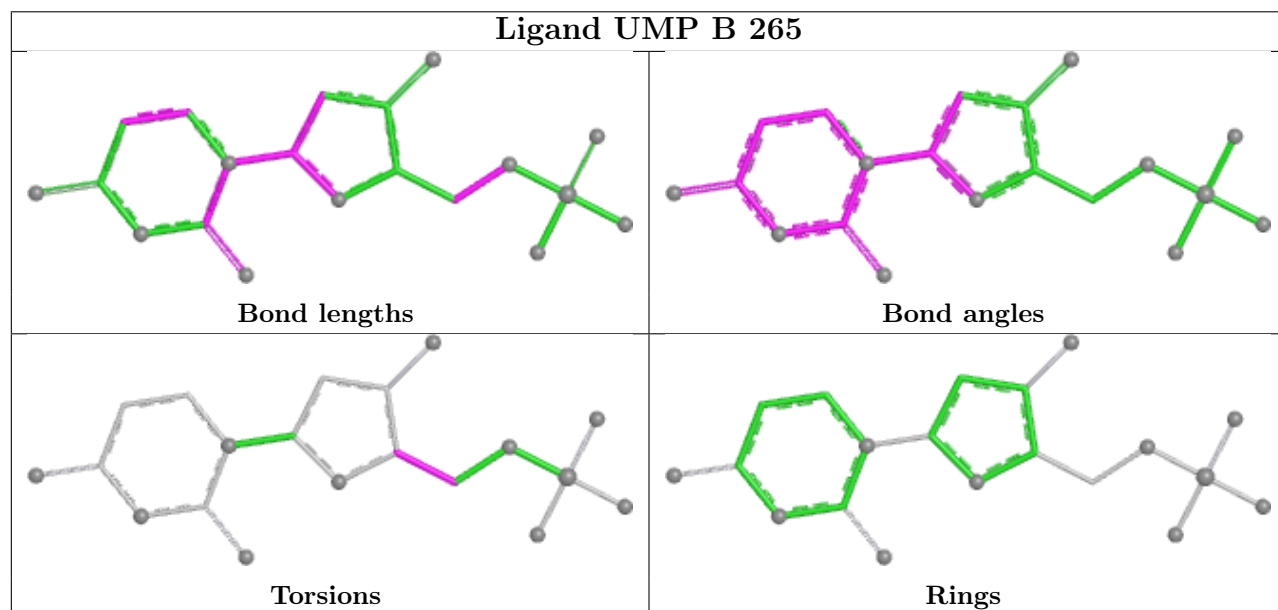
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	266	CB3	1	0
3	A	266	CB3	3	0

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.

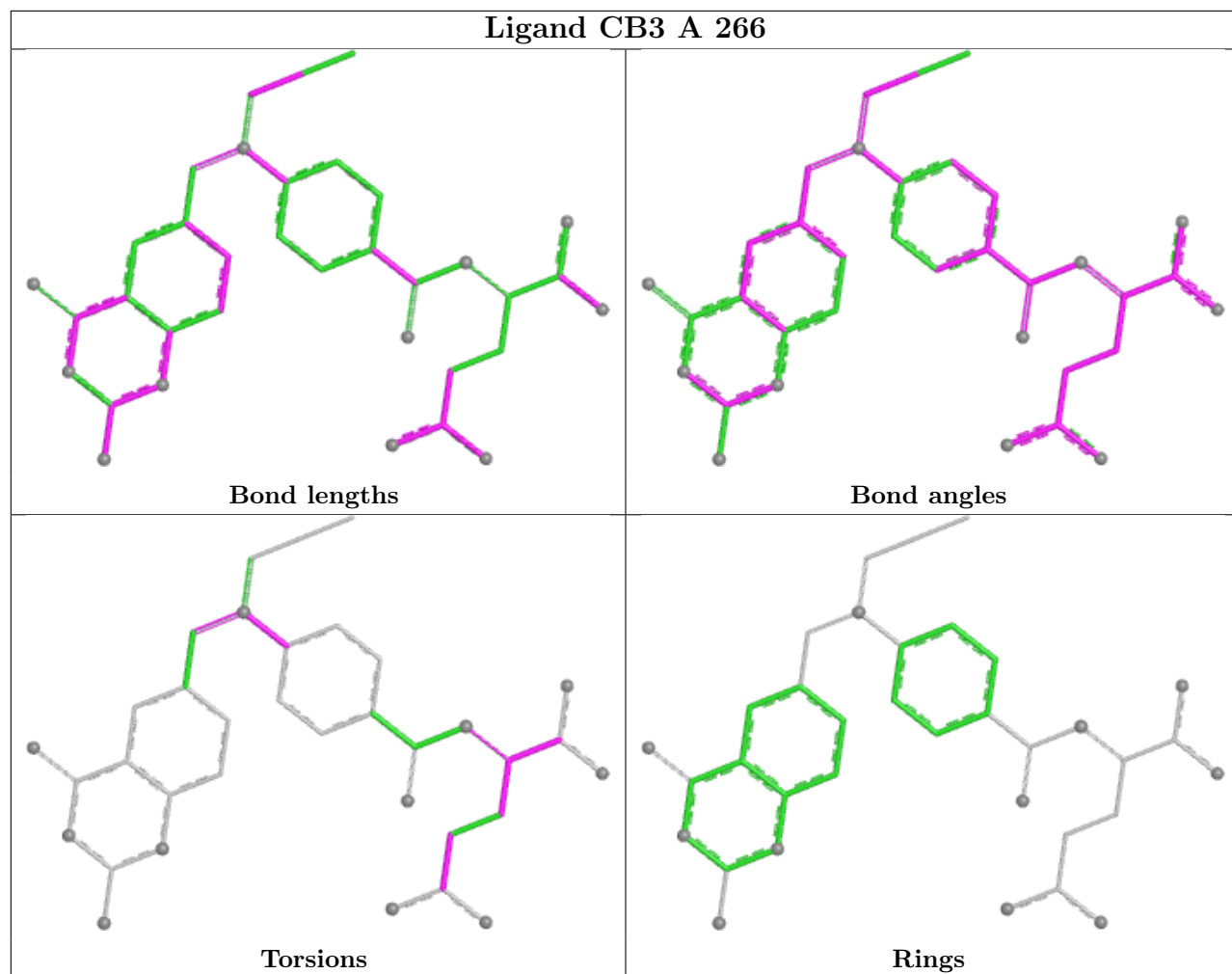
Ligand CB3 B 266



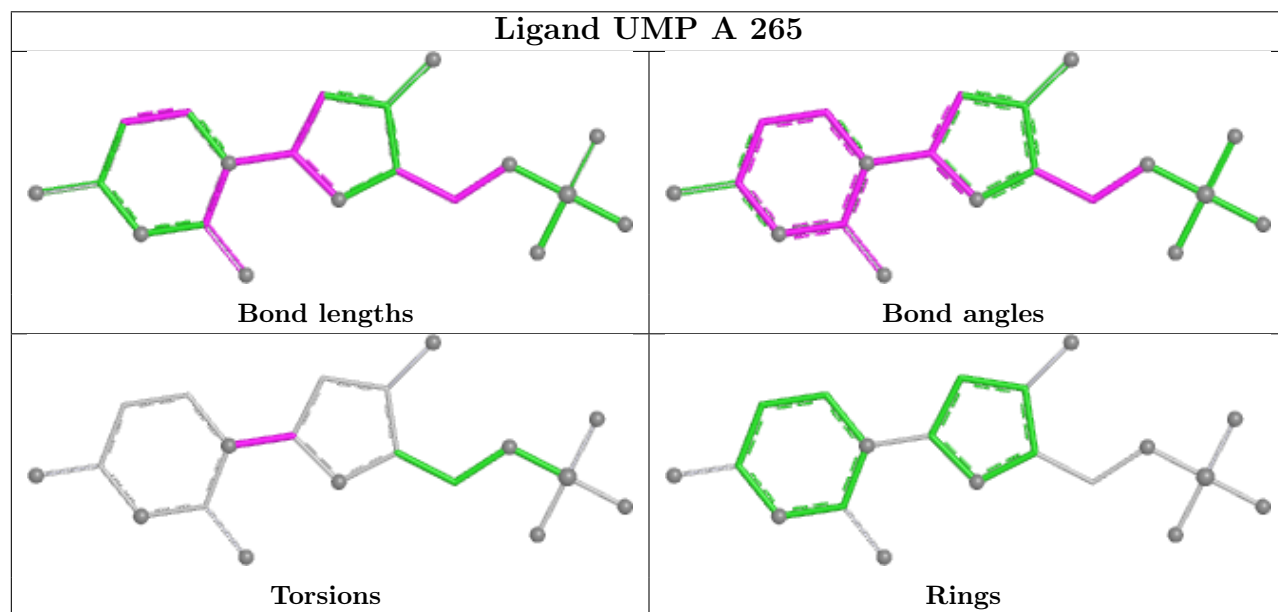
Ligand UMP B 265



Ligand CB3 A 266



Ligand UMP A 265



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.