



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:04 PM UTC

PDB ID : 6QMM / pdb_00006qmm
Title : Crystal structure of Synecochoccus Spermidine Synthase in complex with putrescine, spermidine and MTA
Authors : Guedez, G.; Pothipongsa, A.; Incharoensakdi, A.; Salminen, T.A.
Deposited on : 2019-02-07
Resolution : 2.18 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

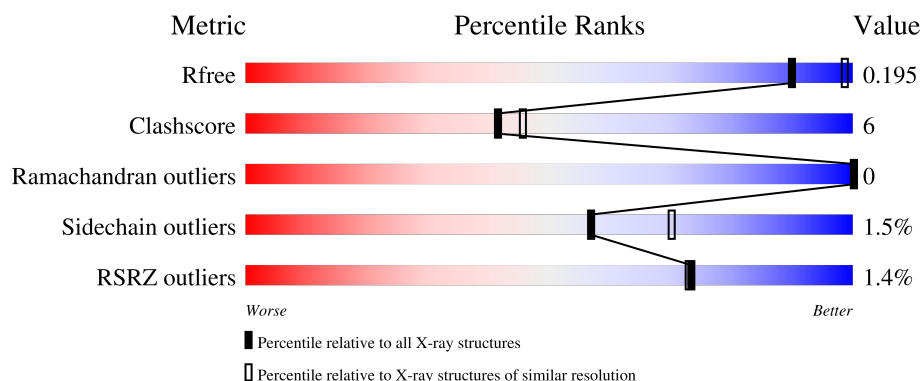
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	281	% 75% 22% ..
2	B	280	% 70% 28% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SPD	B	301	-	-	X	-
5	MTA	B	302	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4728 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.

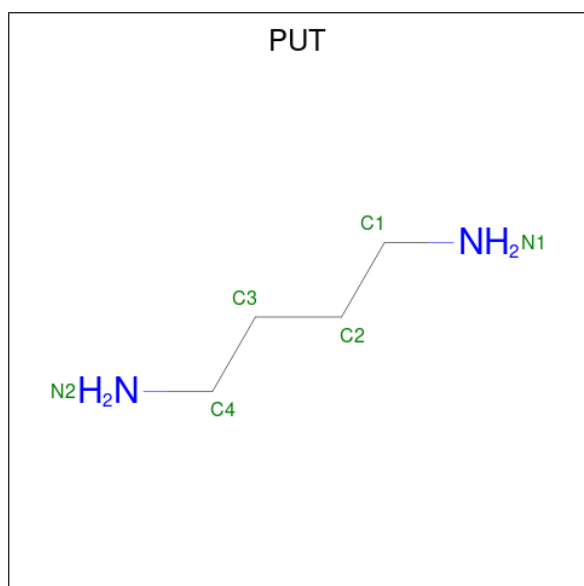
- Molecule 1 is a protein called Polyamine aminopropyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2197	1404	372	414	7			

- Molecule 2 is a protein called Polyamine aminopropyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	280	Total	C	N	O	S	0	0	0
			2214	1416	375	416	7			

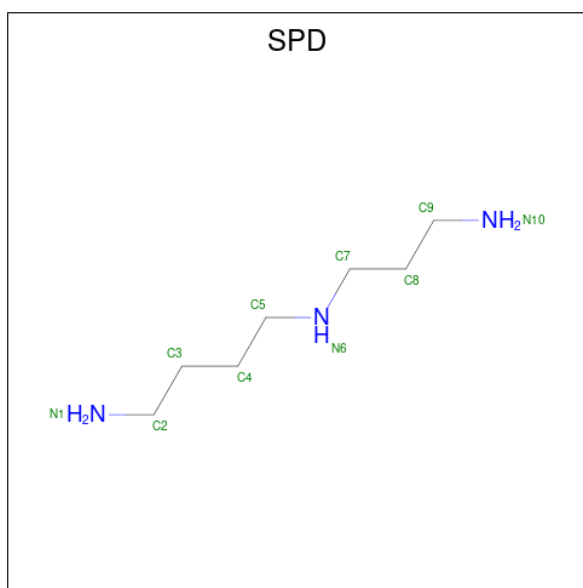
- Molecule 3 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			6	4	2		

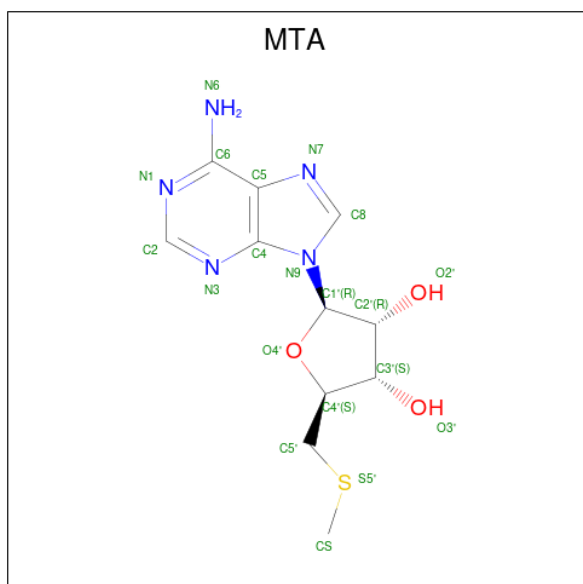
- Molecule 4 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of

Interest" by depositor).



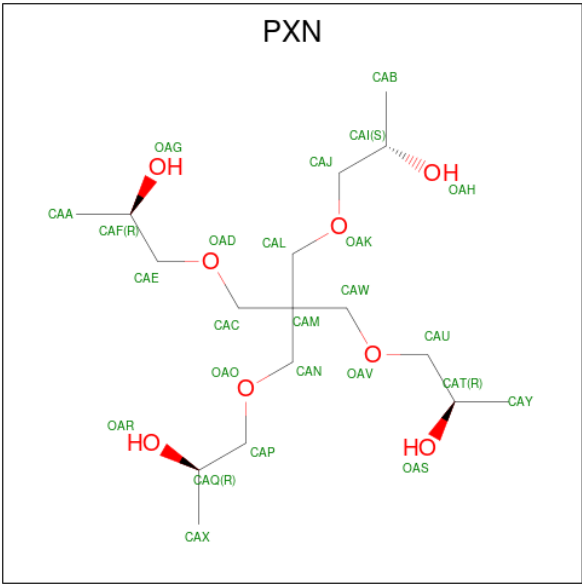
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			10	7	3		

- Molecule 5 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 6 is (2S)-1-[3-{{[(2R)-2-hydroxypropyl]oxy}-2,2-bis({[(2R)-2-hydroxypropyl]oxy}methyl)propoxy]propan-2-ol (CCD ID: PXN) (formula: C₁₇H₃₆O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			25	17	8		

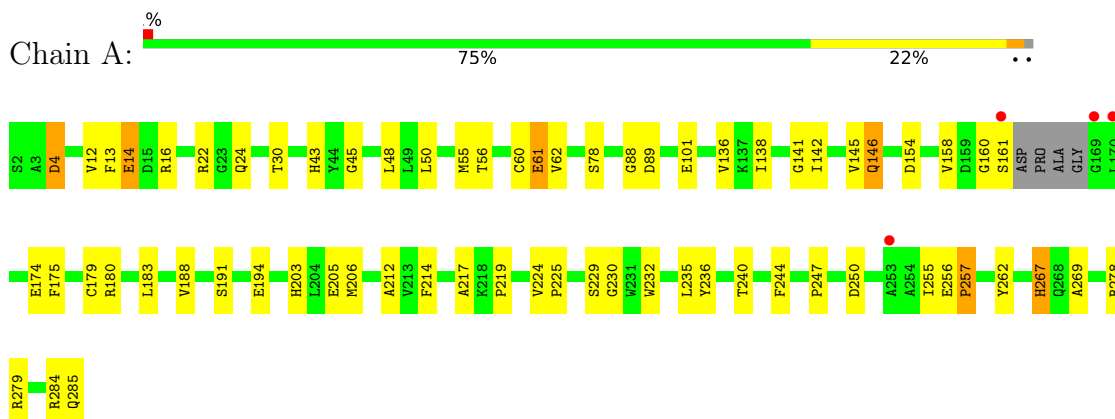
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	125	Total	O	0	0
			125	125		
7	B	131	Total	O	0	0
			131	131		

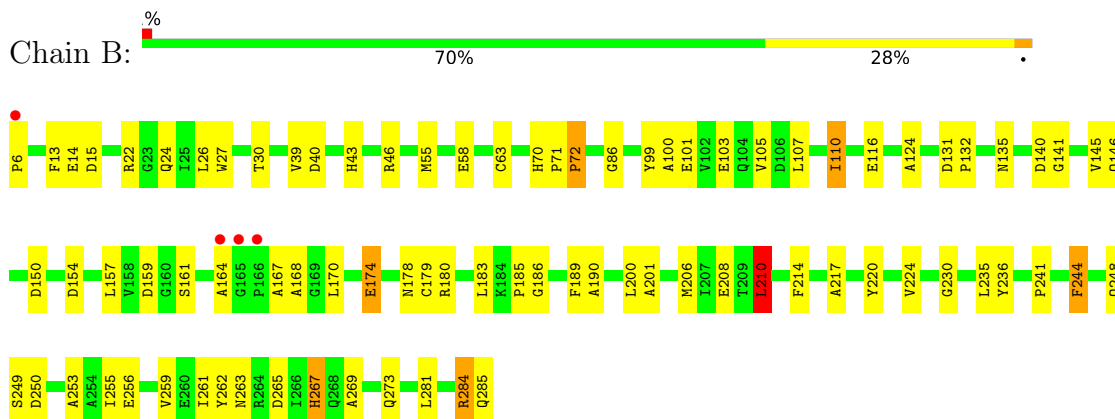
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Polyamine aminopropyltransferase



• Molecule 2: Polyamine aminopropyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.64Å 63.82Å 73.50Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	48.17 – 2.18 48.17 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.17-2.18) 98.3 (48.17-2.18)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.142 , 0.191 (Not available) , 0.195	Depositor DCC
R_{free} test set	1375 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4728	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PXN, MTA, SPD, PUT

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	1.61	28/2255 (1.2%)	1.61	18/3074 (0.6%)
2	B	1.67	41/2275 (1.8%)	1.68	36/3104 (1.2%)
All	All	1.64	69/4530 (1.5%)	1.65	54/6178 (0.9%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	PRO	C-O	-10.50	1.10	1.24
1	A	279	ARG	C-O	-9.73	1.12	1.24
2	B	267	HIS	CE1-NE2	8.86	1.41	1.32
2	B	168	ALA	C-O	8.60	1.33	1.24
2	B	124	ALA	C-O	-8.02	1.13	1.24
1	A	160	GLY	C-O	8.01	1.33	1.24
2	B	180	ARG	C-O	-7.80	1.14	1.24
2	B	256	GLU	CD-OE2	7.78	1.40	1.25
2	B	157	LEU	C-O	7.31	1.32	1.24
2	B	135	ASN	C-O	7.29	1.32	1.24
2	B	190	ALA	C-O	7.18	1.32	1.23
1	A	22	ARG	C-O	6.98	1.32	1.23
1	A	4	ASP	CG-OD2	6.96	1.38	1.25
1	A	247	PRO	C-O	-6.82	1.16	1.23
2	B	103	GLU	C-O	-6.77	1.15	1.24
2	B	72	PRO	C-O	-6.76	1.16	1.24
1	A	205	GLU	C-O	-6.65	1.16	1.24
2	B	145	VAL	C-O	-6.64	1.15	1.24
2	B	256	GLU	C-O	-6.59	1.18	1.24
2	B	116	GLU	C-O	-6.50	1.16	1.24
2	B	201	ALA	C-O	-6.50	1.16	1.24
1	A	136	VAL	C-O	-6.45	1.17	1.24
1	A	229	SER	C-O	6.39	1.32	1.24
2	B	39	VAL	C-O	6.33	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	PRO	C-O	-6.32	1.15	1.24
1	A	141	GLY	C-O	6.32	1.31	1.23
1	A	188	VAL	C-O	6.19	1.30	1.24
2	B	26	LEU	C-O	-6.17	1.16	1.24
1	A	212	ALA	C-O	-6.13	1.16	1.24
2	B	259	VAL	C-O	-6.08	1.17	1.24
2	B	267	HIS	CG-ND1	6.05	1.45	1.38
2	B	105	VAL	C-O	6.00	1.30	1.24
2	B	46	ARG	C-O	6.00	1.31	1.23
1	A	45	GLY	C-O	5.97	1.32	1.23
1	A	12	VAL	C-O	-5.90	1.17	1.24
2	B	249	SER	C-O	-5.87	1.17	1.24
2	B	220	TYR	C-O	-5.79	1.16	1.23
2	B	154	ASP	C-O	-5.74	1.16	1.24
2	B	141	GLY	C-O	5.72	1.30	1.23
1	A	183	LEU	C-O	-5.71	1.16	1.23
2	B	27	TRP	C-O	5.69	1.31	1.23
1	A	214	PHE	C-O	5.58	1.30	1.23
2	B	101	GLU	CD-OE2	5.53	1.35	1.25
2	B	70	HIS	CE1-NE2	5.50	1.38	1.32
1	A	43	HIS	CE1-NE2	5.50	1.38	1.32
1	A	278	ARG	NE-CZ	5.48	1.39	1.33
1	A	4	ASP	C-O	-5.46	1.17	1.24
2	B	43	HIS	CE1-NE2	5.45	1.38	1.32
1	A	219	PRO	C-O	-5.39	1.17	1.23
1	A	88	GLY	C-O	5.38	1.30	1.23
2	B	100	ALA	C-O	-5.37	1.17	1.24
2	B	63	CYS	C-O	-5.35	1.17	1.24
2	B	58	GLU	C-O	-5.35	1.17	1.24
2	B	24	GLN	C-O	5.34	1.30	1.23
2	B	103	GLU	CD-OE2	-5.31	1.15	1.25
2	B	140	ASP	C-O	-5.24	1.17	1.24
1	A	138	ILE	C-O	-5.24	1.17	1.23
1	A	62	VAL	C-O	-5.21	1.17	1.24
1	A	267	HIS	CD2-NE2	-5.19	1.32	1.37
2	B	179	CYS	C-O	5.15	1.30	1.24
1	A	180	ARG	C-O	-5.14	1.18	1.24
2	B	150	ASP	C-O	-5.14	1.17	1.23
1	A	16	ARG	C-O	-5.12	1.17	1.24
1	A	174	GLU	C-O	-5.11	1.18	1.24
2	B	14	GLU	CD-OE1	5.07	1.34	1.25
2	B	265	ASP	C-O	-5.06	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	40	ASP	CG-OD1	5.05	1.34	1.25
1	A	203	HIS	CD2-NE2	5.01	1.43	1.37
2	B	183	LEU	C-O	5.00	1.29	1.23

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ARG	CG-CD-NE	-8.67	92.92	112.00
1	A	4	ASP	CA-CB-CG	8.54	121.14	112.60
2	B	284	ARG	CG-CD-NE	-7.56	95.38	112.00
1	A	22	ARG	NE-CZ-NH2	7.55	125.99	119.20
1	A	61	GLU	N-CA-CB	-7.30	98.16	110.49
1	A	146	GLN	CB-CA-C	7.11	124.88	110.38
2	B	284	ARG	NE-CZ-NH1	-6.98	114.52	121.50
1	A	22	ARG	NE-CZ-NH1	-6.93	114.57	121.50
2	B	146	GLN	CB-CA-C	6.76	123.14	110.63
1	A	61	GLU	CB-CA-C	6.66	123.67	110.42
2	B	249	SER	CA-C-O	-6.47	113.69	120.55
1	A	146	GLN	CB-CG-CD	6.40	123.49	112.60
1	A	278	ARG	NE-CZ-NH2	6.39	124.95	119.20
2	B	30	THR	CB-CA-C	6.35	120.60	110.19
2	B	180	ARG	CA-C-N	6.27	128.68	120.28
2	B	180	ARG	C-N-CA	6.27	128.68	120.28
2	B	200	LEU	CA-C-O	-6.22	114.29	120.82
2	B	140	ASP	CA-CB-CG	6.11	118.71	112.60
2	B	250	ASP	CA-CB-CG	6.09	118.69	112.60
2	B	6	PRO	CA-N-CD	-6.09	103.47	112.00
2	B	70	HIS	CB-CA-C	6.01	122.00	110.17
2	B	248	GLN	CA-C-N	5.99	128.30	120.28
2	B	248	GLN	C-N-CA	5.99	128.30	120.28
2	B	185	PRO	CB-CA-C	-5.91	104.20	111.64
2	B	13	PHE	CA-C-N	5.88	130.48	122.07
2	B	13	PHE	C-N-CA	5.88	130.48	122.07
2	B	244	PHE	CA-CB-CG	5.85	119.65	113.80
2	B	253	ALA	CA-C-O	-5.61	113.52	119.97
2	B	145	VAL	CA-C-O	-5.61	114.42	120.47
2	B	273	GLN	CB-CA-C	-5.52	102.53	109.31
2	B	210	LEU	CA-C-N	5.50	128.20	120.28
2	B	210	LEU	C-N-CA	5.50	128.20	120.28
2	B	174	GLU	CB-CG-CD	5.49	121.94	112.60
2	B	261	ILE	CA-C-N	5.49	128.67	120.87
2	B	261	ILE	C-N-CA	5.49	128.67	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	160	GLY	CA-C-O	-5.47	116.26	121.62
1	A	89	ASP	N-CA-C	-5.46	106.57	113.18
1	A	30	THR	CB-CA-C	5.45	119.01	110.19
2	B	131	ASP	CA-C-O	5.39	124.83	119.49
2	B	214	PHE	CA-C-O	-5.39	115.09	121.66
1	A	247	PRO	N-CA-CB	5.36	108.32	103.33
1	A	14	GLU	CA-C-O	-5.30	114.23	120.81
2	B	285	GLN	CA-C-O	-5.29	111.81	120.80
1	A	284	ARG	CG-CD-NE	-5.27	100.40	112.00
2	B	24	GLN	CB-CA-C	5.27	120.39	109.38
2	B	241	PRO	N-CA-CB	5.21	107.96	103.27
1	A	179	CYS	N-CA-C	-5.16	105.65	111.28
2	B	15	ASP	CA-CB-CG	-5.16	107.44	112.60
2	B	178	ASN	CA-C-O	-5.14	114.98	120.42
2	B	13	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	24	GLN	CB-CG-CD	5.07	121.21	112.60
2	B	263	ASN	CA-C-O	-5.06	115.90	121.31
2	B	178	ASN	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2197	0	2107	26	0
2	B	2214	0	2126	27	0
3	A	6	0	12	2	0
4	B	10	0	19	7	0
5	B	20	0	15	5	0
6	B	25	0	36	3	0
7	A	125	0	0	4	0
7	B	131	0	0	4	0
All	All	4728	0	4315	56	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 6.

All (56) 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)
2:B:186:GLY:H	6:B:303:PXN:HAY	1.31	0.95
2:B:206:MET:HE2	2:B:235:LEU:HD12	1.65	0.79
4:B:301:SPD:H72	5:B:302:MTA:H5'2	1.67	0.76
2:B:110:ILE:HD12	7:B:484:HOH:O	1.85	0.76
2:B:210:LEU:HD23	2:B:235:LEU:HD13	1.74	0.68
2:B:244:PHE:O	2:B:267:HIS:HE1	1.80	0.64
4:B:301:SPD:H72	5:B:302:MTA:C5'	2.27	0.63
2:B:86:GLY:O	2:B:107:LEU:HD11	2.00	0.62
1:A:101:GLU:HG3	7:A:472:HOH:O	2.01	0.61
1:A:250:ASP:HB2	7:A:510:HOH:O	2.01	0.60
1:A:244:PHE:O	1:A:267:HIS:HE1	1.85	0.59
1:A:262:TYR:OH	1:A:267:HIS:HD2	1.85	0.59
4:B:301:SPD:N1	7:B:401:HOH:O	2.32	0.58
1:A:55:MET:HE1	3:A:301:PUT:H12	1.84	0.58
2:B:167:ALA:O	2:B:170:LEU:HB2	2.04	0.56
2:B:161:SER:HA	4:B:301:SPD:H41	1.88	0.56
1:A:262:TYR:OH	1:A:267:HIS:CD2	2.59	0.56
2:B:55:MET:HB3	5:B:302:MTA:CS	2.35	0.56
1:A:224:VAL:O	1:A:230:GLY:HA2	2.06	0.55
2:B:208:GLU:OE2	2:B:284:ARG:HD3	2.08	0.53
2:B:186:GLY:N	6:B:303:PXN:HAY	2.12	0.53
2:B:186:GLY:H	6:B:303:PXN:CAY	2.15	0.53
1:A:158:VAL:HB	1:A:191:SER:HB3	1.91	0.52
1:A:78:SER:O	1:A:154:ASP:HB3	2.10	0.52
2:B:262:TYR:OH	2:B:267:HIS:HD2	1.94	0.49
4:B:301:SPD:H92	5:B:302:MTA:HCS2	1.94	0.49
1:A:13:PHE:CE2	1:A:14:GLU:HG3	2.47	0.48
1:A:146:GLN:HE21	1:A:175:PHE:HA	1.78	0.48
2:B:224:VAL:O	2:B:230:GLY:HA2	2.14	0.48
1:A:4:ASP:OD1	7:A:401:HOH:O	2.20	0.47
1:A:50:LEU:HD12	1:A:55:MET:HG3	1.97	0.47
1:A:269:ALA:HB1	2:B:269:ALA:HB1	1.97	0.47
2:B:71:PRO:HB2	2:B:72:PRO:HD3	1.96	0.46
1:A:256:GLU:N	1:A:257:PRO:CD	2.79	0.46
2:B:164:ALA:C	7:B:423:HOH:O	2.58	0.45
2:B:161:SER:HA	4:B:301:SPD:C4	2.46	0.45
1:A:158:VAL:HB	1:A:191:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:MET:HB3	5:B:302:MTA:HCS2	1.99	0.45
1:A:206:MET:HE2	1:A:206:MET:HB3	1.85	0.45
1:A:48:LEU:HB3	1:A:56:THR:HG22	1.98	0.44
1:A:60:CYS:SG	1:A:225:PRO:HD2	2.58	0.44
2:B:99:TYR:CZ	2:B:255:ILE:HG13	2.54	0.43
1:A:101:GLU:CG	7:A:472:HOH:O	2.63	0.42
2:B:281:LEU:O	2:B:284:ARG:HB2	2.19	0.42
2:B:174:GLU:H	2:B:174:GLU:CD	2.27	0.42
1:A:255:ILE:HA	1:A:255:ILE:HD12	1.84	0.42
1:A:217:ALA:HA	1:A:236:TYR:O	2.19	0.42
1:A:194:GLU:HA	1:A:232:TRP:CZ2	2.55	0.42
2:B:110:ILE:CD1	7:B:484:HOH:O	2.55	0.42
1:A:145:VAL:HG21	1:A:175:PHE:CE1	2.55	0.41
1:A:232:TRP:CZ2	3:A:301:PUT:H41	2.55	0.41
2:B:159:ASP:OD1	4:B:301:SPD:H81	2.20	0.41
2:B:262:TYR:OH	2:B:267:HIS:CD2	2.72	0.41
1:A:142:ILE:O	1:A:146:GLN:HG3	2.21	0.41
2:B:217:ALA:HA	2:B:236:TYR:O	2.19	0.40
2:B:189:PHE:CD1	2:B:189:PHE:C	2.99	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	273/281 (97%)	259 (95%)	14 (5%)	0	100	100
2	B	278/280 (99%)	264 (95%)	14 (5%)	0	100	100
All	All	551/561 (98%)	523 (95%)	28 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	229/231 (99%)	225 (98%)	4 (2%)	53	66
2	B	230/230 (100%)	227 (99%)	3 (1%)	61	74
All	All	459/461 (100%)	452 (98%)	7 (2%)	57	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLU
1	A	161	SER
1	A	235	LEU
1	A	285	GLN
2	B	22	ARG
2	B	110	ILE
2	B	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	146	GLN
1	A	243	GLN
1	A	267	HIS
2	B	146	GLN
2	B	243	GLN
2	B	258	GLN
2	B	267	HIS
2	B	273	GLN

5.3.3 RNA

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$
6	PXN	B	303	-	24,24,24	0.94	1 (4%)	30,30,30	1.70	5 (16%)
4	SPD	B	301	-	9,9,9	0.91	1 (11%)	8,8,8	1.11	0
3	PUT	A	301	-	5,5,5	0.21	0	4,4,4	0.84	0
5	MTA	B	302	-	22,22,22	3.11	12 (54%)	32,32,32	3.43	22 (68%)

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
6	PXN	B	303	-	-	12/28/28/28	-
4	SPD	B	301	-	-	5/7/7/7	-
3	PUT	A	301	-	-	2/3/3/3	-
5	MTA	B	302	-	-	1/7/23/23	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	MTA	C5-C4	7.00	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	MTA	O4'-C1'	6.14	1.56	1.42
5	B	302	MTA	C5'-S5'	5.61	1.94	1.81
5	B	302	MTA	C8-N7	4.61	1.40	1.31
5	B	302	MTA	C2-N3	3.56	1.40	1.33
5	B	302	MTA	C5-C6	3.32	1.50	1.41
5	B	302	MTA	C1'-N9	3.04	1.54	1.46
5	B	302	MTA	O2'-C2'	2.60	1.49	1.43
5	B	302	MTA	C3'-C2'	2.55	1.60	1.53
5	B	302	MTA	C6-N6	2.54	1.40	1.34
4	B	301	SPD	C8-C7	-2.26	1.42	1.51
5	B	302	MTA	C2-N1	2.17	1.37	1.33
6	B	303	PXN	OAV-CAW	2.13	1.47	1.42
5	B	302	MTA	C2'-C1'	2.03	1.59	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	302	MTA	C5-C4-N3	-8.78	114.63	126.72
5	B	302	MTA	O4'-C4'-C5'	7.43	127.96	108.83
5	B	302	MTA	N3-C4-N9	5.59	136.68	127.17
5	B	302	MTA	O4'-C1'-N9	4.99	117.67	108.09
6	B	303	PXN	CAC-OAD-CAE	-4.81	98.50	113.08
5	B	302	MTA	C4-C5-N7	-4.77	105.12	110.58
5	B	302	MTA	O3'-C3'-C4'	-4.48	98.22	111.08
5	B	302	MTA	C2-N3-C4	4.36	122.48	111.83
6	B	303	PXN	CAW-OAV-CAU	-3.98	101.01	113.08
5	B	302	MTA	O3'-C3'-C2'	3.52	123.12	111.82
5	B	302	MTA	C6-C5-C4	3.48	121.94	117.18
5	B	302	MTA	C5-N7-C8	3.11	108.33	103.45
6	B	303	PXN	OAK-CAJ-CAI	3.03	118.72	109.34
5	B	302	MTA	C4'-C5'-S5'	-2.86	104.38	113.89
5	B	302	MTA	O2'-C2'-C3'	2.77	120.70	111.82
5	B	302	MTA	C2'-C3'-C4'	2.70	107.82	102.61
5	B	302	MTA	N3-C2-N1	-2.68	124.53	128.58
5	B	302	MTA	O4'-C1'-C2'	-2.66	100.91	106.62
5	B	302	MTA	O2'-C2'-C1'	2.65	119.25	110.10
5	B	302	MTA	C5-C4-N9	2.62	108.66	105.81
5	B	302	MTA	C5'-C4'-C3'	-2.41	109.03	115.06
5	B	302	MTA	C2'-C1'-N9	2.39	119.25	113.30
5	B	302	MTA	N6-C6-N1	2.35	123.60	118.38
5	B	302	MTA	C3'-C2'-C1'	-2.33	97.06	101.46
6	B	303	PXN	OAR-CAQ-CAX	2.15	118.72	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	303	PXN	OAO-CAN-CAM	2.13	114.52	108.84
5	B	302	MTA	C4-N9-C1'	2.10	131.55	126.63

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	303	PXN	OAK-CAL-CAM-CAW
6	B	303	PXN	OAK-CAL-CAM-CAN
6	B	303	PXN	OAD-CAC-CAM-CAN
6	B	303	PXN	OAK-CAL-CAM-CAC
6	B	303	PXN	OAD-CAC-CAM-CAW
6	B	303	PXN	OAD-CAC-CAM-CAL
3	A	301	PUT	N1-C1-C2-C3
6	B	303	PXN	CAM-CAN-OAO-CAP
6	B	303	PXN	CAF-CAE-OAD-CAC
6	B	303	PXN	CAQ-CAP-OAO-CAN
6	B	303	PXN	CAM-CAC-OAD-CAE
4	B	301	SPD	C7-C8-C9-N10
6	B	303	PXN	CAM-CAL-OAK-CAJ
4	B	301	SPD	C4-C5-N6-C7
4	B	301	SPD	C3-C4-C5-N6
3	A	301	PUT	C2-C3-C4-N2
4	B	301	SPD	C2-C3-C4-C5
5	B	302	MTA	C4'-C5'-S5'-CS
4	B	301	SPD	N1-C2-C3-C4
6	B	303	PXN	CAI-CAJ-OAK-CAL

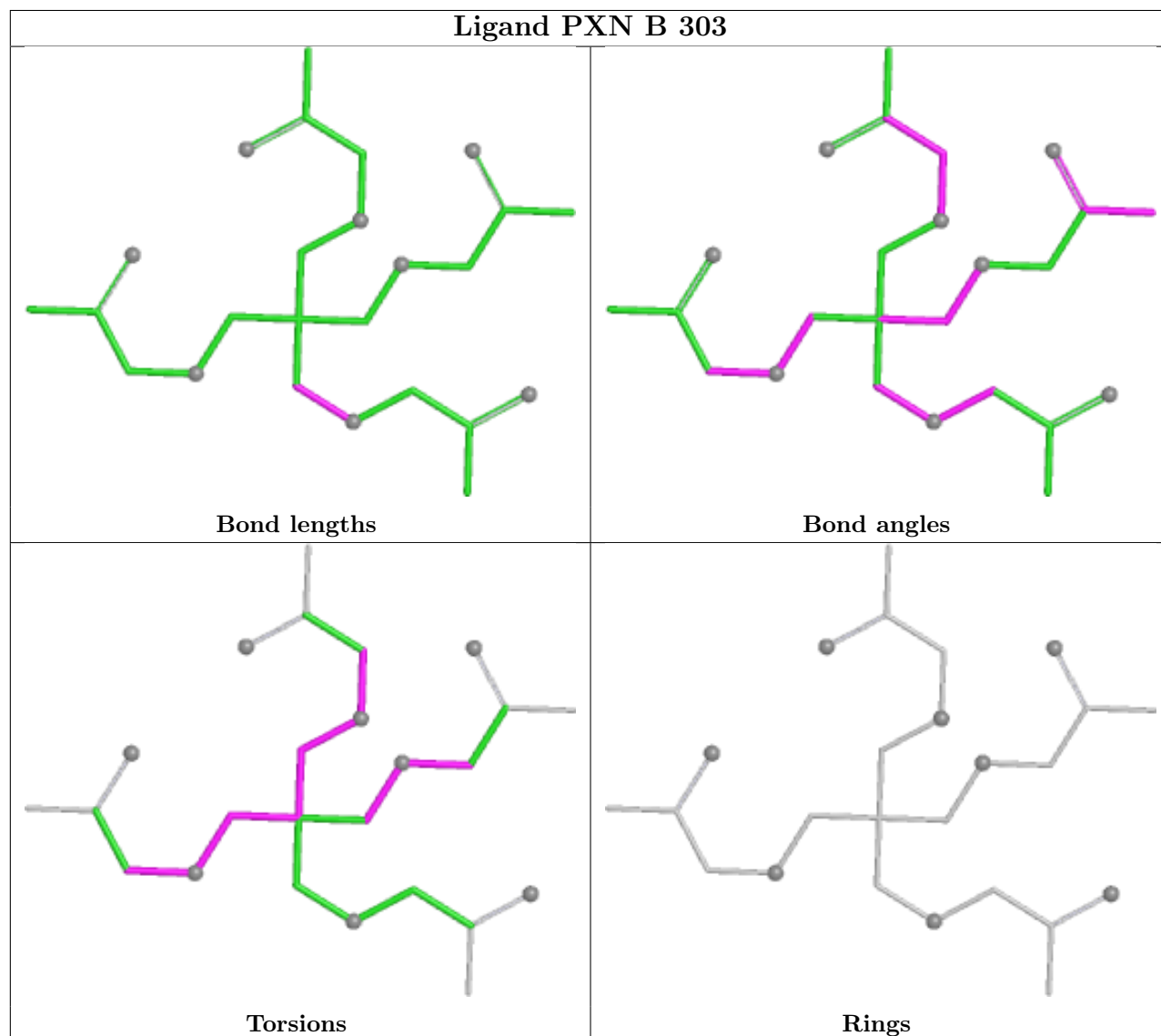
There are no ring outliers.

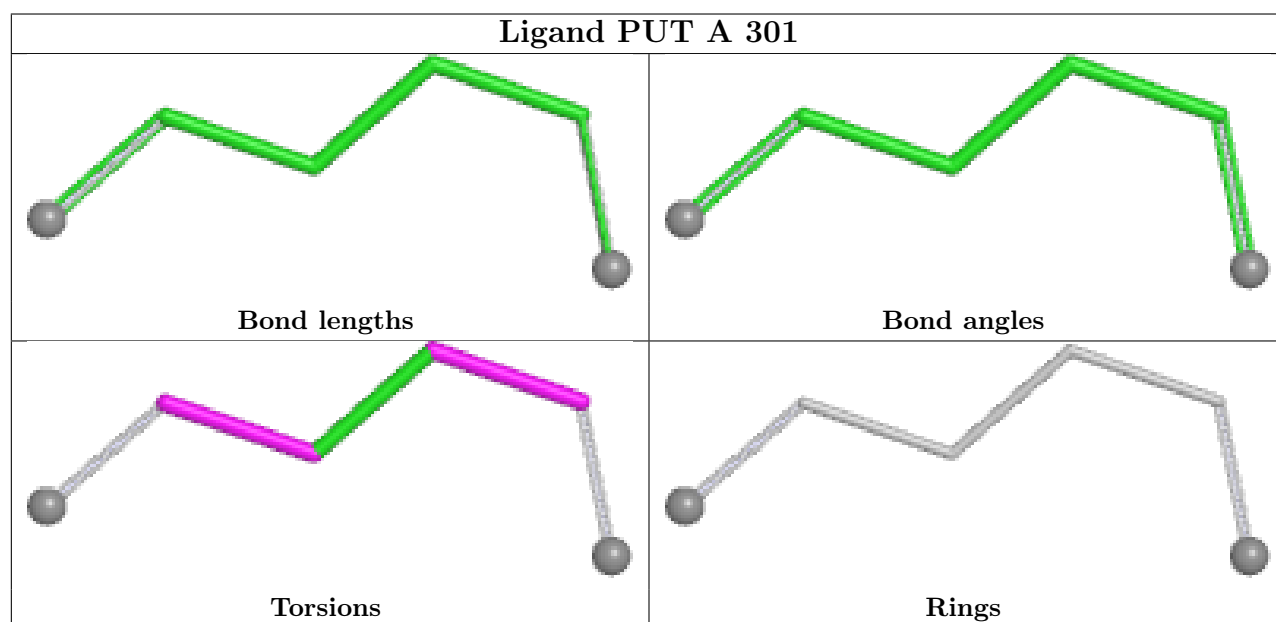
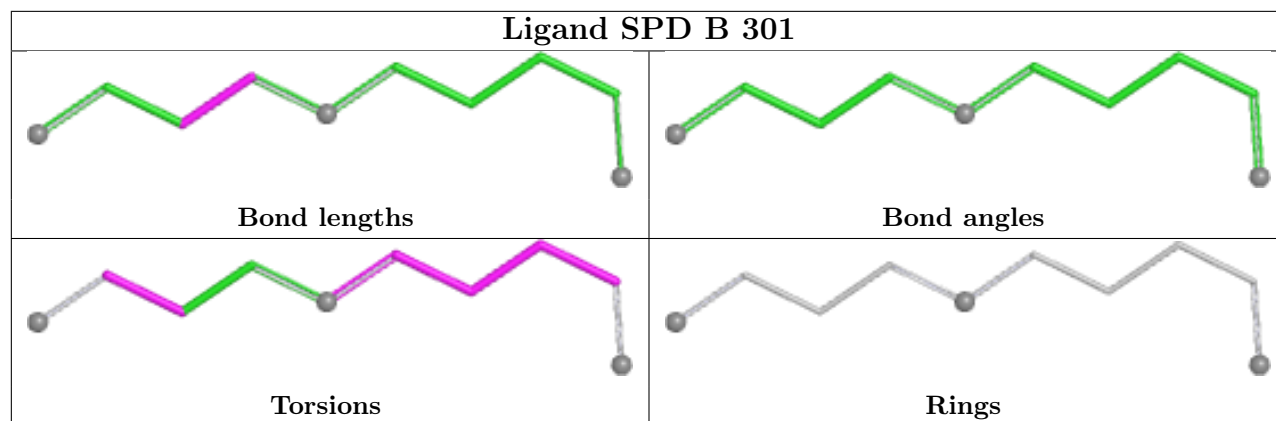
4 monomers are involved in 14 short contacts:

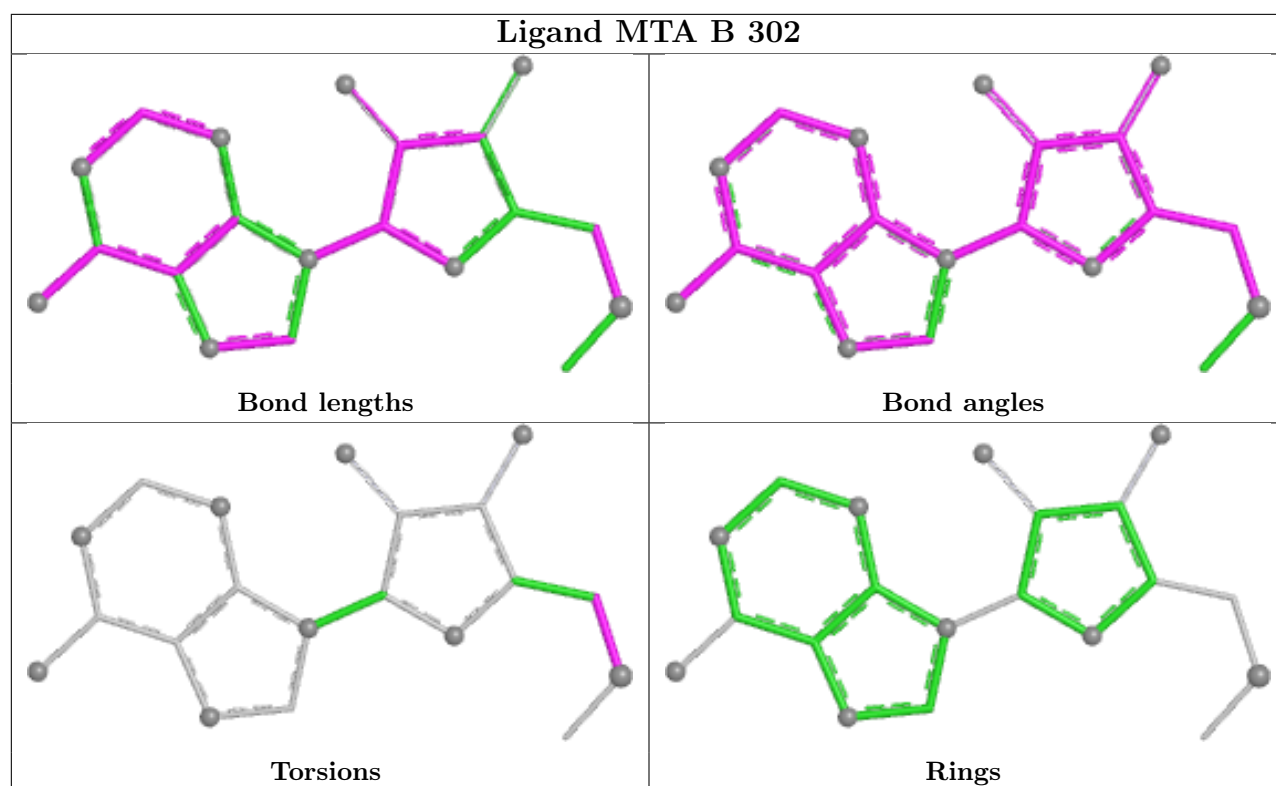
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	PXN	3	0
4	B	301	SPD	7	0
3	A	301	PUT	2	0
5	B	302	MTA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/281 (98%)	-0.32	4 (1%) 73 73	10, 19, 31, 52	1 (0%)
2	B	280/280 (100%)	-0.44	4 (1%) 73 73	7, 15, 31, 68	2 (0%)
All	All	557/561 (99%)	-0.38	8 (1%) 73 73	7, 17, 31, 68	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	165	GLY	5.5
2	B	164	ALA	3.6
1	A	170	LEU	3.1
1	A	169	GLY	2.9
1	A	253	ALA	2.6
2	B	166	PRO	2.5
2	B	6	PRO	2.3
1	A	161	SER	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

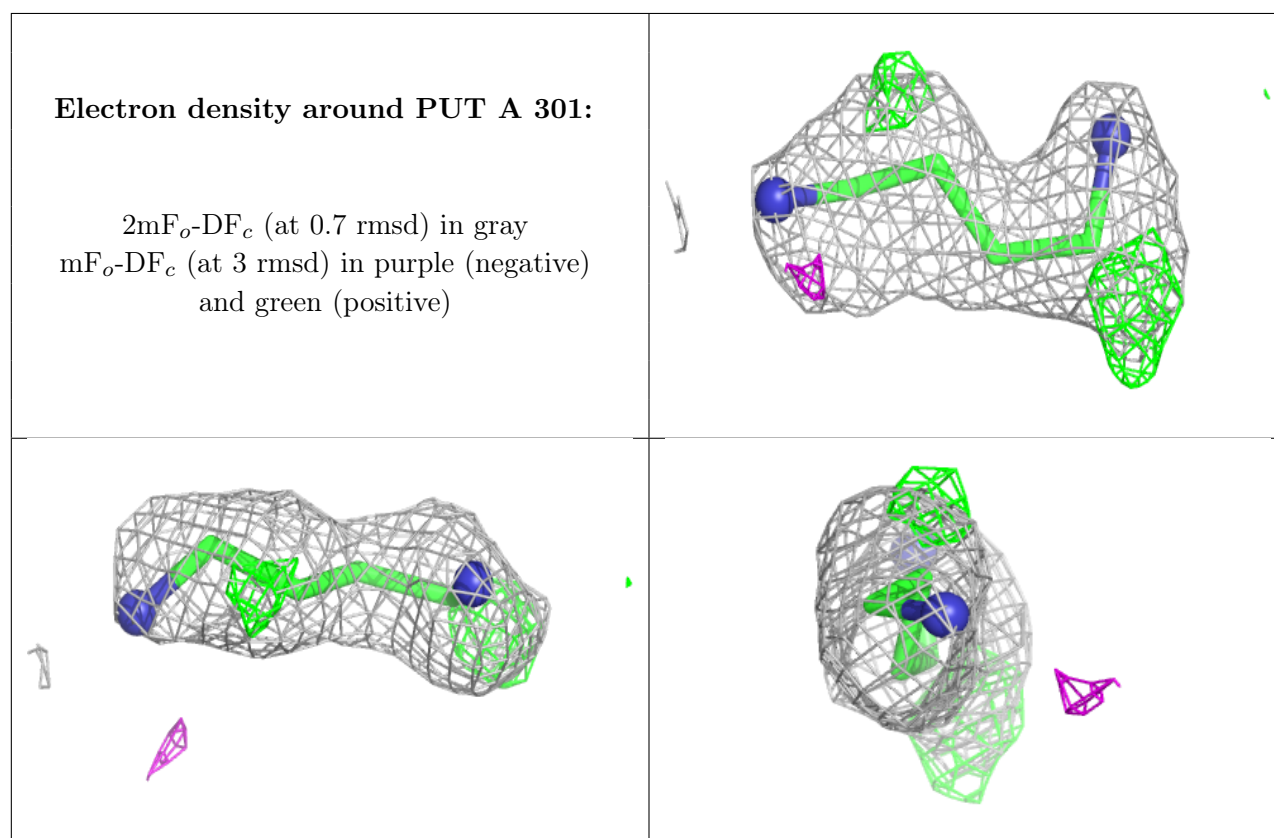
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

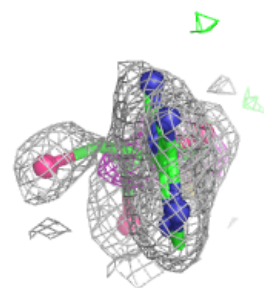
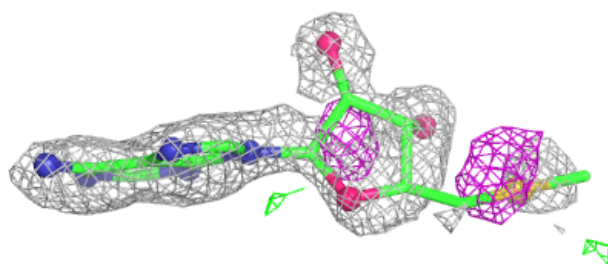
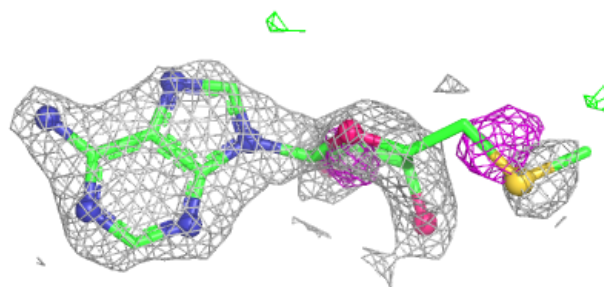
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PUT	A	301	6/6	0.81	0.20	40,43,46,48	0
5	MTA	B	302	20/20	0.84	0.12	31,37,57,59	0
6	PXN	B	303	25/25	0.87	0.13	20,39,55,62	0
4	SPD	B	301	10/10	0.89	0.12	22,26,31,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



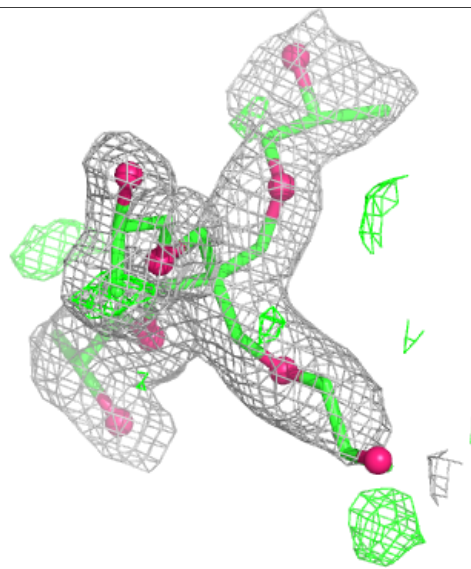
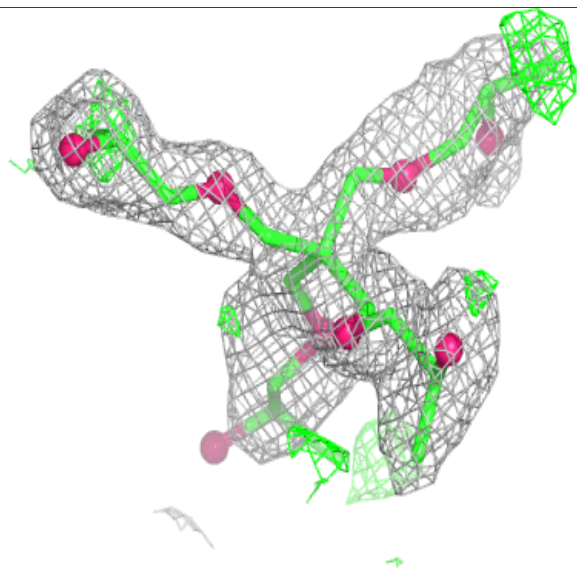
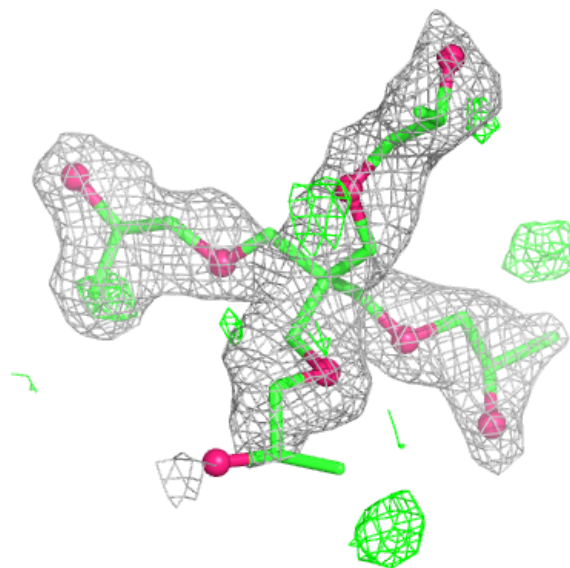
Electron density around MTA B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



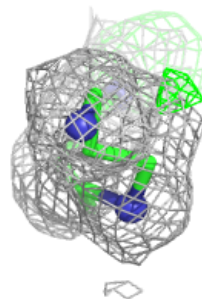
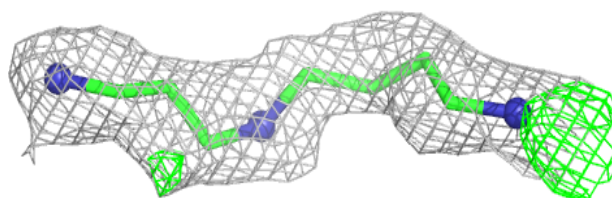
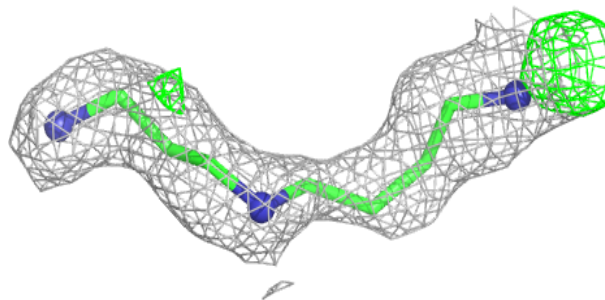
Electron density around PXN B 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SPD B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.