



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 09:31 AM EDT

PDB ID : 3FPJ  
Title : Crystal Structure of E81Q mutant of MtNAS in complex with S-ADENOSYLMETHIONINE  
Authors : Dreyfus, C.; Pignol, D.; Arnoux, P.  
Deposited on : 2009-01-05  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

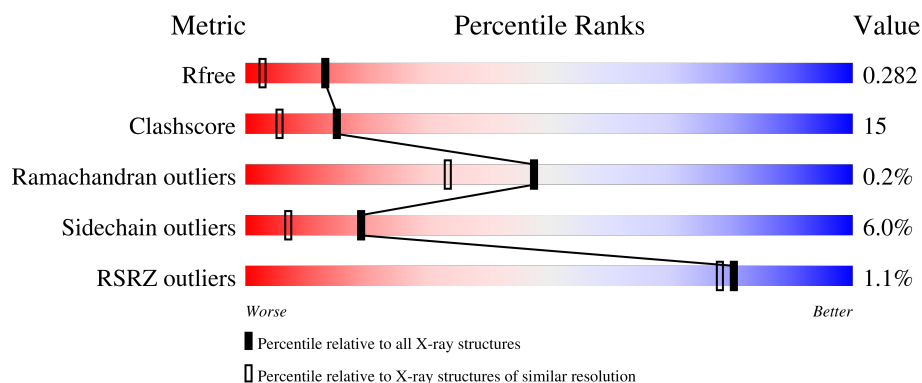
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

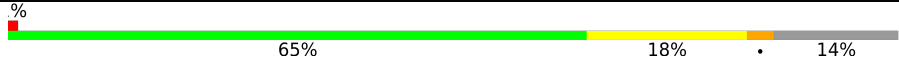

The reported resolution of this entry is 1.80 Å.

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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	298	
1	B	298	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4826 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			2050	1309	350	380	11			
1	B	265	Total	C	N	O	S	0	6	0
			2160	1378	370	400	12			

There are 66 discrepancies between the modelled and reference sequences:

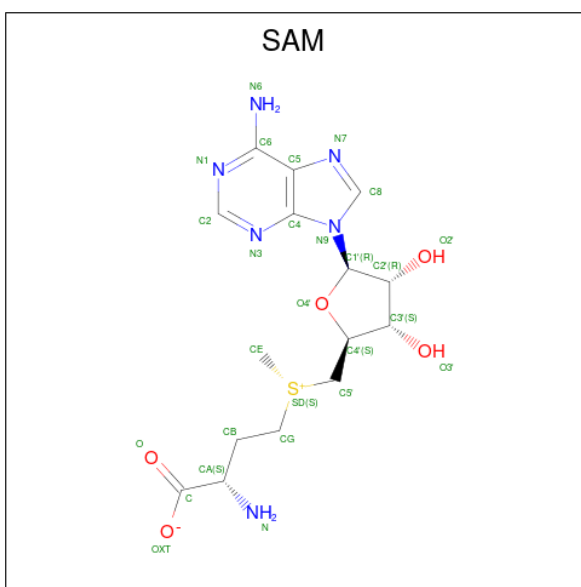
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLN	GLU	engineered mutation	UNP O26771
A	267	LYS	-	expression tag	UNP O26771
A	268	GLY	-	expression tag	UNP O26771
A	269	GLU	-	expression tag	UNP O26771
A	270	LEU	-	expression tag	UNP O26771
A	271	ASN	-	expression tag	UNP O26771
A	272	SER	-	expression tag	UNP O26771
A	273	LYS	-	expression tag	UNP O26771
A	274	LEU	-	expression tag	UNP O26771
A	275	GLU	-	expression tag	UNP O26771
A	276	GLY	-	expression tag	UNP O26771
A	277	LYS	-	expression tag	UNP O26771
A	278	PRO	-	expression tag	UNP O26771
A	279	ILE	-	expression tag	UNP O26771
A	280	PRO	-	expression tag	UNP O26771
A	281	ASN	-	expression tag	UNP O26771
A	282	PRO	-	expression tag	UNP O26771
A	283	LEU	-	expression tag	UNP O26771
A	284	LEU	-	expression tag	UNP O26771
A	285	GLY	-	expression tag	UNP O26771
A	286	LEU	-	expression tag	UNP O26771
A	287	ASP	-	expression tag	UNP O26771
A	288	SER	-	expression tag	UNP O26771
A	289	THR	-	expression tag	UNP O26771
A	290	ARG	-	expression tag	UNP O26771

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	THR	-	expression tag	UNP O26771
A	292	GLY	-	expression tag	UNP O26771
A	293	HIS	-	expression tag	UNP O26771
A	294	HIS	-	expression tag	UNP O26771
A	295	HIS	-	expression tag	UNP O26771
A	296	HIS	-	expression tag	UNP O26771
A	297	HIS	-	expression tag	UNP O26771
A	298	HIS	-	expression tag	UNP O26771
B	81	GLN	GLU	engineered mutation	UNP O26771
B	267	LYS	-	expression tag	UNP O26771
B	268	GLY	-	expression tag	UNP O26771
B	269	GLU	-	expression tag	UNP O26771
B	270	LEU	-	expression tag	UNP O26771
B	271	ASN	-	expression tag	UNP O26771
B	272	SER	-	expression tag	UNP O26771
B	273	LYS	-	expression tag	UNP O26771
B	274	LEU	-	expression tag	UNP O26771
B	275	GLU	-	expression tag	UNP O26771
B	276	GLY	-	expression tag	UNP O26771
B	277	LYS	-	expression tag	UNP O26771
B	278	PRO	-	expression tag	UNP O26771
B	279	ILE	-	expression tag	UNP O26771
B	280	PRO	-	expression tag	UNP O26771
B	281	ASN	-	expression tag	UNP O26771
B	282	PRO	-	expression tag	UNP O26771
B	283	LEU	-	expression tag	UNP O26771
B	284	LEU	-	expression tag	UNP O26771
B	285	GLY	-	expression tag	UNP O26771
B	286	LEU	-	expression tag	UNP O26771
B	287	ASP	-	expression tag	UNP O26771
B	288	SER	-	expression tag	UNP O26771
B	289	THR	-	expression tag	UNP O26771
B	290	ARG	-	expression tag	UNP O26771
B	291	THR	-	expression tag	UNP O26771
B	292	GLY	-	expression tag	UNP O26771
B	293	HIS	-	expression tag	UNP O26771
B	294	HIS	-	expression tag	UNP O26771
B	295	HIS	-	expression tag	UNP O26771
B	296	HIS	-	expression tag	UNP O26771
B	297	HIS	-	expression tag	UNP O26771
B	298	HIS	-	expression tag	UNP O26771

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).

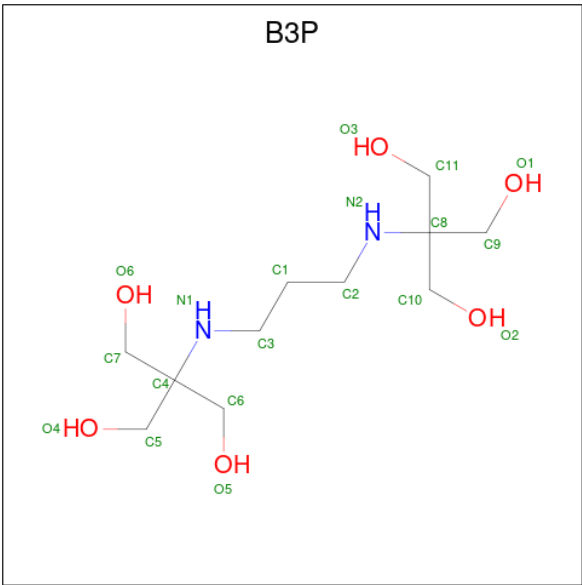


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Br	0	0
			2	2		
3	B	1	Total	Br	0	0
			1	1		

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: C<sub>11</sub>H<sub>26</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			19	11	2	6		

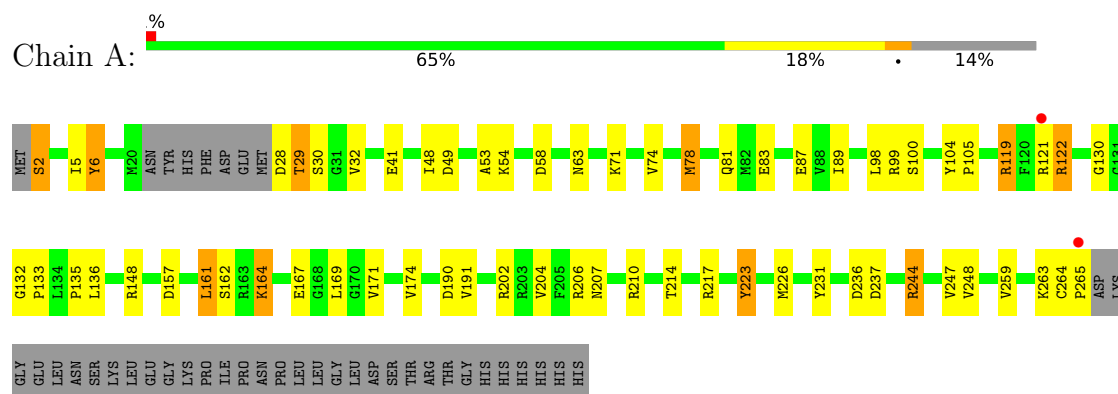
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		
5	B	296	Total	O	0	0
			296	296		

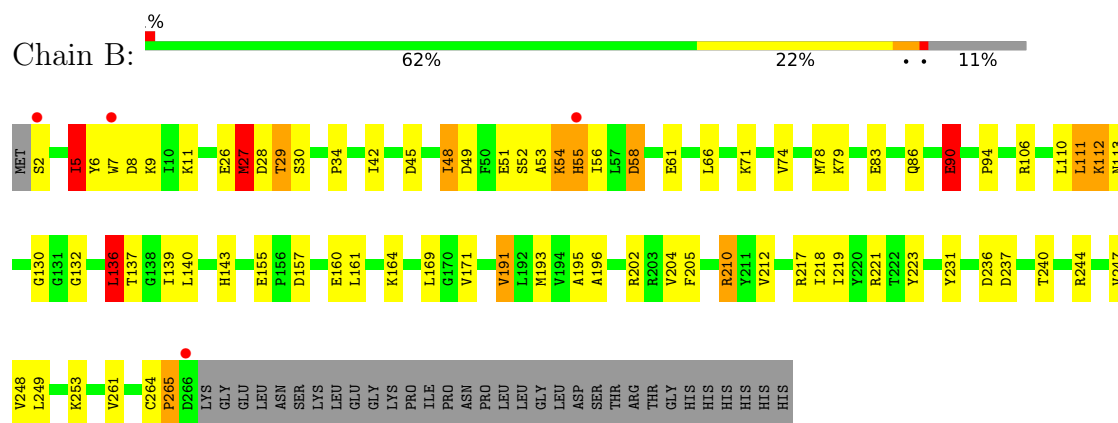
### 3 Residue-property plots

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: Putative uncharacterized protein



#### • Molecule 1: Putative uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.60Å 68.98Å 147.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 1.80 29.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.80-1.80) 99.4 (29.80-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.225 , 0.284 0.225 , 0.282	Depositor DCC
$R_{free}$ test set	3082 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, SAM, BR

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	1.24	5/2091 (0.2%)	1.11	8/2826 (0.3%)
1	B	1.34	5/2218 (0.2%)	1.19	12/2998 (0.4%)
All	All	1.29	10/4309 (0.2%)	1.15	20/5824 (0.3%)

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	1
1	B	0	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	LYS	CD-CE	6.76	1.68	1.51
1	A	6	TYR	CB-CG	-6.24	1.42	1.51
1	A	248	VAL	CB-CG1	5.72	1.64	1.52
1	A	204	VAL	CB-CG1	5.66	1.64	1.52
1	B	112	LYS	CE-NZ	5.44	1.62	1.49
1	A	164	LYS	CD-CE	5.30	1.64	1.51
1	B	90	GLU	CB-CG	-5.20	1.42	1.52
1	B	205	PHE	CE2-CZ	5.18	1.47	1.37
1	B	204	VAL	CB-CG1	5.07	1.63	1.52
1	A	223	TYR	CE2-CZ	5.03	1.45	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	B	210	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	B	110	LEU	CB-CG-CD2	-8.13	97.18	111.00
1	A	2	SER	N-CA-C	7.98	132.55	111.00
1	B	136	LEU	CB-CG-CD2	7.72	124.12	111.00
1	A	122	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	B	27	MET	CG-SD-CE	-7.30	88.51	100.20
1	A	217	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	49	ASP	CB-CG-OD1	6.95	124.56	118.30
1	B	27	MET	CB-CA-C	-6.34	97.71	110.40
1	B	191	VAL	CG1-CB-CG2	6.25	120.90	110.90
1	A	190	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	B	58	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	244	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	99	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	217	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	28	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	B	66	LEU	CB-CG-CD2	-5.24	102.10	111.00
1	B	5	ILE	CB-CA-C	-5.14	101.32	111.60
1	B	217	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	CYS	Peptide
1	B	264	CYS	Peptide
1	B	265	PRO	Peptide

## 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	2050	0	2066	57	0
1	B	2160	0	2166	73	0
2	A	27	0	22	5	0
2	B	27	0	22	5	0
3	A	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	B	19	0	26	0	0
5	A	244	0	0	26	0
5	B	296	0	0	33	0
All	All	4826	0	4302	130	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 15.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HB3	5:A:445:HOH:O	1.24	1.28
1:A:237:ASP:HB3	5:A:338:HOH:O	1.49	1.13
1:B:157:ASP:HB2	5:B:332:HOH:O	1.46	1.13
1:A:133:PRO:HA	5:A:526:HOH:O	1.49	1.12
1:B:30:SER:HB2	5:B:549:HOH:O	1.48	1.12
1:A:119:ARG:NH1	1:A:121:ARG:HG2	1.66	1.08
1:A:119:ARG:HH11	1:A:121:ARG:HG2	1.14	1.07
1:B:8:ASP:HB2	5:B:547:HOH:O	1.53	1.06
1:B:45:ASP:HB3	5:B:527:HOH:O	1.58	1.04
1:B:48:ILE:CG2	5:B:527:HOH:O	2.15	0.93
1:B:48:ILE:HG21	5:B:527:HOH:O	1.70	0.92
1:A:53:ALA:HA	1:A:226:MET:HE1	1.53	0.90
1:B:29:THR:HG21	1:B:83:GLU:OE1	1.72	0.90
1:A:53:ALA:HA	1:A:226:MET:CE	2.05	0.87
1:B:155:GLU:OE1	5:B:458:HOH:O	1.93	0.86
1:A:244:ARG:HD3	1:B:52:SER:OG	1.77	0.85
1:B:90:GLU:HG3	5:B:347:HOH:O	1.77	0.83
1:B:143:HIS:HB2	5:B:511:HOH:O	1.81	0.79
1:A:5:ILE:CD1	5:A:438:HOH:O	2.30	0.78
1:B:244[A]:ARG:HH21	1:B:247:VAL:HG21	1.46	0.78
1:A:236:ASP:HB2	5:A:345:HOH:O	1.86	0.75
1:A:78[B]:MET:HG2	5:A:302:HOH:O	1.85	0.74
1:B:111:LEU:HG	5:B:478:HOH:O	1.88	0.73
1:B:171:VAL:HG13	5:B:511:HOH:O	1.89	0.73
1:A:157:ASP:HB2	5:A:584:HOH:O	1.89	0.73
1:A:28:ASP:N	5:A:429:HOH:O	2.22	0.72
1:A:161:LEU:HA	1:A:164:LYS:HE3	1.71	0.72
1:B:7:TRP:NE1	1:B:11:LYS:HE2	2.04	0.72
1:A:265:PRO:HB2	5:A:372:HOH:O	1.90	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HB3	5:A:526:HOH:O	1.90	0.71
1:B:7:TRP:HE1	1:B:11:LYS:HE2	1.56	0.70
1:A:78[B]:MET:HE2	1:A:81:GLN:NE2	2.07	0.70
1:B:244[A]:ARG:HH21	1:B:247:VAL:CG2	2.05	0.69
1:A:236:ASP:HB3	1:B:55[A]:HIS:NE2	2.08	0.68
1:B:6:TYR:CE1	1:B:42:ILE:HG12	2.30	0.67
1:B:48:ILE:HD12	1:B:52:SER:HB2	1.78	0.66
1:B:237:ASP:O	1:B:240[A]:THR:HG23	1.94	0.66
1:B:160[B]:GLU:HG2	5:B:504:HOH:O	1.97	0.65
1:B:160[B]:GLU:OE1	1:B:164:LYS:NZ	2.29	0.65
1:B:74:VAL:O	1:B:78[B]:MET:HG3	1.96	0.65
1:B:237:ASP:HB2	5:B:553:HOH:O	1.97	0.64
1:B:27:MET:HA	5:B:554:HOH:O	1.97	0.63
1:A:171:VAL:HG12	5:A:528:HOH:O	1.98	0.62
1:A:214:THR:HG21	1:A:265:PRO:HD3	1.82	0.61
1:A:5:ILE:HD11	5:A:438:HOH:O	1.99	0.59
1:B:171:VAL:CG1	5:B:511:HOH:O	2.48	0.59
1:B:112:LYS:CE	5:B:433:HOH:O	2.51	0.59
1:B:140:LEU:HB3	5:B:478:HOH:O	2.02	0.59
1:A:226:MET:CE	1:A:226:MET:HA	2.33	0.58
1:A:89:ILE:HD11	1:A:161:LEU:CD2	2.33	0.58
1:B:5:ILE:HG13	5:B:406:HOH:O	2.03	0.58
1:B:29:THR:CG2	5:B:606:HOH:O	2.51	0.58
1:A:63:ASN:HB2	5:A:440:HOH:O	2.03	0.57
1:B:111:LEU:HD21	1:B:137:THR:HG23	1.86	0.57
1:A:78[B]:MET:CG	5:A:302:HOH:O	2.49	0.56
1:B:132:GLY:CA	2:B:301:SAM:H5'1	2.36	0.56
1:B:202:ARG:HD3	5:B:469:HOH:O	2.06	0.55
1:B:112:LYS:HE3	5:B:433:HOH:O	2.06	0.54
1:A:100:SER:HB3	5:A:340:HOH:O	2.07	0.54
1:B:112:LYS:HD3	5:B:385:HOH:O	2.07	0.54
1:A:78[B]:MET:CE	1:A:81:GLN:NE2	2.71	0.54
1:A:100:SER:CB	5:A:340:HOH:O	2.56	0.54
1:A:5:ILE:HD11	5:A:366:HOH:O	2.07	0.53
1:B:171:VAL:HG22	5:B:511:HOH:O	2.07	0.53
1:A:174:VAL:HG23	5:A:528:HOH:O	2.08	0.53
1:A:122:ARG:HG2	5:A:312:HOH:O	2.10	0.52
1:A:89:ILE:CD1	1:A:161:LEU:CD2	2.88	0.52
1:B:113:ASN:HB3	1:B:248:VAL:HG11	1.91	0.51
1:B:48:ILE:HD11	1:B:53:ALA:N	2.26	0.51
1:A:202:ARG:NH1	5:A:496:HOH:O	2.43	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASP:OD1	5:B:483:HOH:O	2.20	0.49
1:B:52:SER:O	1:B:56:ILE:HG13	2.12	0.49
1:A:29:THR:HG21	1:A:83:GLU:OE1	2.12	0.48
1:A:104:TYR:HB3	1:A:105:PRO:HD3	1.95	0.48
1:B:27:MET:HB2	1:B:79:LYS:HD2	1.94	0.48
1:A:148:ARG:HD3	5:A:385:HOH:O	2.13	0.48
1:A:247:VAL:HG22	1:A:259:VAL:HG13	1.96	0.48
1:A:207:ASN:ND2	1:A:210:ARG:HH11	2.12	0.47
1:A:6:TYR:CE1	1:A:48:ILE:HD11	2.49	0.47
1:B:49:ASP:OD1	1:B:51:GLU:HB2	2.14	0.47
1:A:98:LEU:HD22	1:A:169:LEU:HD11	1.97	0.47
1:A:214:THR:HG22	1:A:263:LYS:O	2.14	0.47
2:A:301:SAM:H8	5:A:494:HOH:O	2.14	0.47
1:B:130:GLY:O	2:B:301:SAM:HE2	2.14	0.47
1:A:226:MET:HB2	1:A:226:MET:HE3	1.92	0.47
1:A:236:ASP:CB	1:B:55[A]:HIS:NE2	2.78	0.47
1:B:244[A]:ARG:HA	1:B:261:VAL:HG12	1.96	0.47
2:A:301:SAM:HE1	2:A:301:SAM:HB1	1.77	0.47
1:B:86:GLN:O	1:B:90:GLU:HG2	2.14	0.47
1:B:244[B]:ARG:HA	1:B:261:VAL:HG12	1.96	0.47
1:A:119:ARG:HD3	5:A:441:HOH:O	2.15	0.46
1:B:48:ILE:CD1	1:B:52:SER:HB2	2.44	0.46
1:B:106:ARG:HD3	1:B:253:LYS:O	2.15	0.46
1:B:49:ASP:OD2	5:B:430:HOH:O	2.21	0.46
1:A:32:VAL:HA	5:A:565:HOH:O	2.16	0.46
1:B:58:ASP:HB2	5:B:510:HOH:O	2.16	0.46
1:A:132:GLY:HA3	2:A:301:SAM:HG1	1.97	0.46
1:B:171:VAL:CG2	5:B:511:HOH:O	2.63	0.46
1:A:78[B]:MET:CE	2:A:301:SAM:H5'1	2.46	0.46
1:B:94:PRO:HB2	1:B:169:LEU:HD23	1.98	0.45
1:B:29:THR:HG23	5:B:606:HOH:O	2.15	0.45
1:B:132:GLY:HA3	2:B:301:SAM:H5'1	1.98	0.45
1:B:136:LEU:HD22	1:B:140:LEU:HG	1.97	0.45
1:B:2:SER:HB3	1:B:55[B]:HIS:CE1	2.51	0.45
1:B:244[A]:ARG:NH2	1:B:247:VAL:CG2	2.77	0.45
1:A:148:ARG:CD	5:A:385:HOH:O	2.64	0.45
1:A:130:GLY:O	2:A:301:SAM:HE2	2.17	0.44
1:A:74:VAL:HG22	5:A:302:HOH:O	2.18	0.44
1:B:231:TYR:HD1	5:B:413:HOH:O	2.00	0.44
1:B:212:VAL:HG21	1:B:218:ILE:HD11	1.99	0.44
1:B:193:MET:HA	1:B:219:ILE:O	2.17	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LYS:HE2	5:B:449:HOH:O	2.17	0.44
1:B:244[A]:ARG:HD3	5:B:483:HOH:O	2.17	0.43
1:A:223:TYR:CE1	1:A:231:TYR:HB3	2.53	0.43
1:B:196:ALA:HB2	1:B:221:ARG:HB3	2.01	0.43
1:A:54:LYS:O	1:A:58:ASP:HB2	2.18	0.43
1:A:89:ILE:HD11	1:A:161:LEU:HD22	2.01	0.42
1:A:202:ARG:HG2	1:A:206:ARG:NH1	2.34	0.42
1:B:195:ALA:HB1	2:B:301:SAM:HE1	2.01	0.42
1:A:53:ALA:CA	1:A:226:MET:CE	2.88	0.42
1:B:86:GLN:NE2	5:B:397:HOH:O	2.51	0.42
1:B:139:ILE:HG23	1:B:171:VAL:HG21	2.02	0.42
2:B:301:SAM:HN2	2:B:301:SAM:HG2	1.37	0.42
1:A:135:PRO:HD3	1:A:162:SER:HB2	2.01	0.42
1:B:54:LYS:HB3	1:B:54:LYS:HE3	1.74	0.42
1:B:61:GLU:HB3	5:B:544:HOH:O	2.19	0.41
1:B:249:LEU:HD23	1:B:249:LEU:HA	1.84	0.41
1:A:78[B]:MET:HE2	1:A:81:GLN:CD	2.41	0.41
1:B:223:TYR:CE1	1:B:231:TYR:HB3	2.56	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	254/298 (85%)	247 (97%)	7 (3%)	0	100	100
1	B	269/298 (90%)	261 (97%)	7 (3%)	1 (0%)	34	21
All	All	523/596 (88%)	508 (97%)	14 (3%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	PRO

### 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	223/259 (86%)	211 (95%)	12 (5%)	22	9
1	B	236/259 (91%)	219 (93%)	17 (7%)	14	4
All	All	459/518 (89%)	430 (94%)	29 (6%)	19	6

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	29	THR
1	A	30	SER
1	A	41	GLU
1	A	71	LYS
1	A	78[A]	MET
1	A	78[B]	MET
1	A	87	GLU
1	A	119	ARG
1	A	136	LEU
1	A	161	LEU
1	A	191	VAL
1	B	5	ILE
1	B	9	LYS
1	B	26	GLU
1	B	27	MET
1	B	29	THR
1	B	34	PRO
1	B	48	ILE
1	B	54	LYS
1	B	55[A]	HIS
1	B	55[B]	HIS
1	B	71	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	90	GLU
1	B	111	LEU
1	B	136	LEU
1	B	161	LEU
1	B	191	VAL
1	B	210	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	150	ASN
1	A	175	ASN
1	A	207	ASN
1	B	63	ASN
1	B	64	HIS
1	B	75	ASN
1	B	86	GLN
1	B	113	ASN
1	B	256	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	SAM	A	301	-	21,29,29	4.24	10 (47%)	18,42,42	3.66	9 (50%)
4	B3P	B	302	-	18,18,18	1.63	3 (16%)	21,23,23	2.84	9 (42%)
2	SAM	B	301	-	21,29,29	3.83	10 (47%)	18,42,42	3.30	5 (27%)

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	SAM	A	301	-	-	5/8/33/33	0/3/3/3
4	B3P	B	302	-	-	12/28/28/28	-
2	SAM	B	301	-	-	5/8/33/33	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SAM	C2-N3	11.56	1.50	1.32
2	B	301	SAM	C2-N3	9.68	1.47	1.32
2	B	301	SAM	C2-N1	8.54	1.49	1.33
2	A	301	SAM	C4-N3	7.55	1.46	1.35
2	A	301	SAM	C8-N7	7.53	1.48	1.34
2	A	301	SAM	C2-N1	7.08	1.47	1.33
2	B	301	SAM	C8-N7	7.02	1.47	1.34
2	B	301	SAM	C4-N3	5.87	1.43	1.35
4	B	302	B3P	C10-C8	5.43	1.59	1.53
2	A	301	SAM	O4'-C1'	5.19	1.48	1.41
2	A	301	SAM	C5-C4	4.03	1.51	1.40
2	B	301	SAM	C6-N6	3.44	1.46	1.34
2	B	301	SAM	C5-C4	3.41	1.49	1.40
2	B	301	SAM	O4'-C1'	3.19	1.45	1.41
2	A	301	SAM	C6-C5	2.88	1.54	1.43
2	A	301	SAM	C6-N6	2.76	1.44	1.34
2	B	301	SAM	C6-C5	2.56	1.52	1.43
4	B	302	B3P	O2-C10	2.42	1.50	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SAM	C6-N1	2.36	1.47	1.37
2	B	301	SAM	C6-N1	2.09	1.46	1.37
2	A	301	SAM	C5-N7	2.08	1.47	1.39
2	B	301	SAM	C5-N7	2.03	1.47	1.39
4	B	302	B3P	O6-C7	2.01	1.48	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	SAM	N3-C2-N1	-8.75	115.00	128.68
2	A	301	SAM	C5'-SD-CG	8.73	125.67	103.40
2	B	301	SAM	O4'-C4'-C5'	8.32	129.90	108.88
2	A	301	SAM	O4'-C4'-C5'	7.00	126.58	108.88
2	A	301	SAM	N3-C2-N1	-6.84	117.99	128.68
4	B	302	B3P	O2-C10-C8	6.43	124.66	111.63
4	B	302	B3P	C11-C8-C9	-5.76	97.86	110.04
4	B	302	B3P	C2-N2-C8	4.93	123.07	116.08
2	B	301	SAM	O3'-C3'-C4'	-4.32	98.55	111.05
4	B	302	B3P	C6-C4-C5	3.76	117.98	110.04
2	A	301	SAM	O3'-C3'-C4'	-3.69	100.39	111.05
2	A	301	SAM	C2-N1-C6	3.63	124.97	118.75
4	B	302	B3P	O6-C7-C4	3.61	118.95	111.63
4	B	302	B3P	C3-C1-C2	-3.07	103.04	114.26
2	B	301	SAM	C2-N1-C6	2.86	123.65	118.75
2	A	301	SAM	O4'-C1'-C2'	-2.80	102.83	106.93
4	B	302	B3P	C3-N1-C4	-2.61	112.38	116.08
2	A	301	SAM	C2'-C3'-C4'	2.39	107.29	102.64
2	A	301	SAM	C3'-C2'-C1'	2.38	104.56	100.98
4	B	302	B3P	C11-C8-C10	2.28	114.87	110.04
2	A	301	SAM	O2'-C2'-C1'	2.28	119.27	110.85
4	B	302	B3P	O3-C11-C8	-2.19	107.20	111.63
2	B	301	SAM	O4'-C4'-C3'	2.09	109.25	105.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SAM	C-CA-CB-CG
2	A	301	SAM	CB-CG-SD-CE
2	B	301	SAM	N-CA-CB-CG
2	B	301	SAM	C-CA-CB-CG
2	B	301	SAM	CA-CB-CG-SD

*Continued on next page...*

*Continued from previous page...*

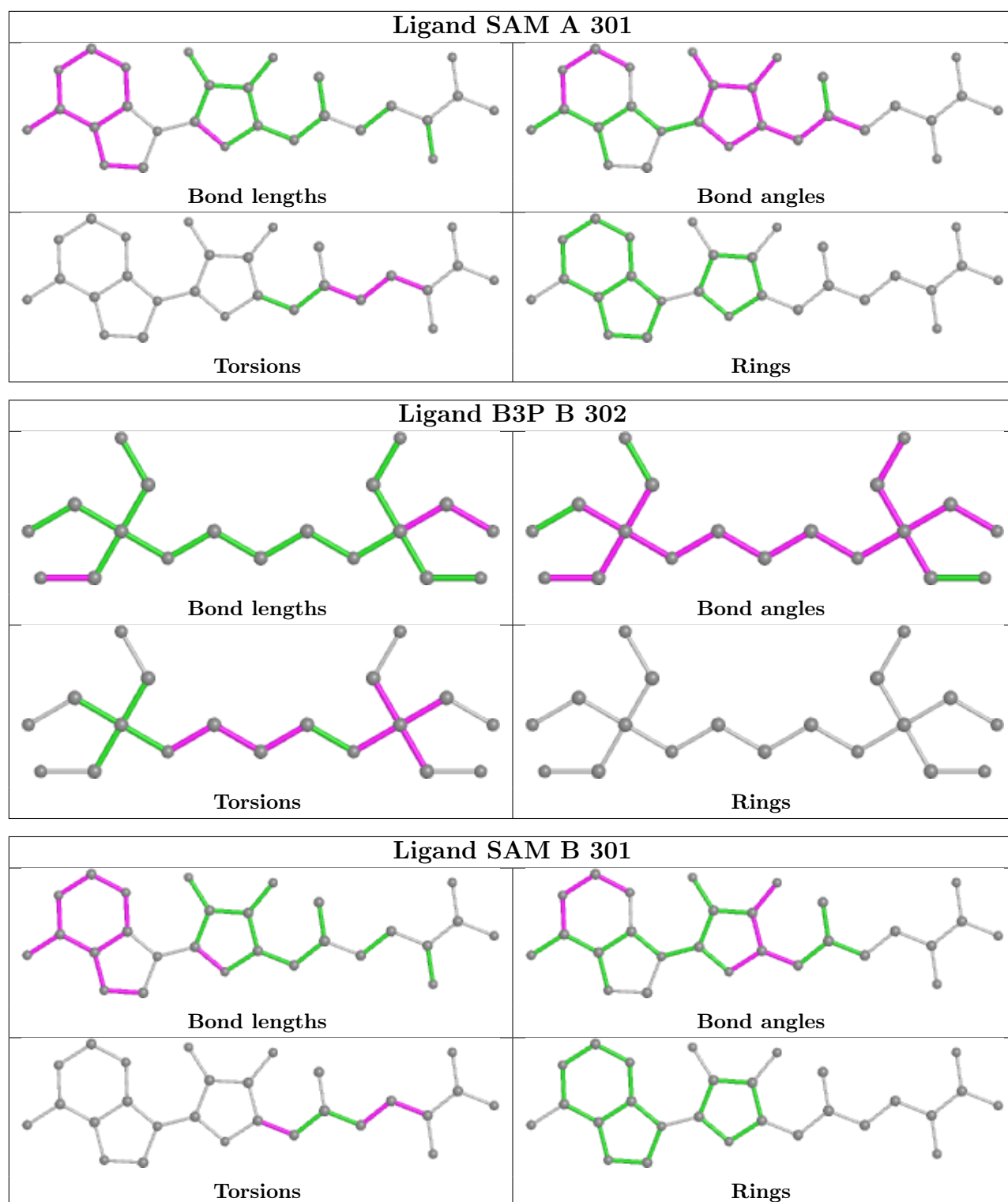
Mol	Chain	Res	Type	Atoms
2	B	301	SAM	O4'-C4'-C5'-SD
2	B	301	SAM	C3'-C4'-C5'-SD
4	B	302	B3P	C9-C8-N2-C2
4	B	302	B3P	C10-C8-N2-C2
4	B	302	B3P	C11-C8-N2-C2
4	B	302	B3P	O2-C10-C8-C9
4	B	302	B3P	C3-C1-C2-N2
4	B	302	B3P	C2-C1-C3-N1
4	B	302	B3P	O3-C11-C8-N2
4	B	302	B3P	C1-C3-N1-C4
4	B	302	B3P	N2-C8-C9-O1
4	B	302	B3P	O3-C11-C8-C9
2	A	301	SAM	N-CA-CB-CG
2	A	301	SAM	CB-CG-SD-C5'
2	A	301	SAM	CA-CB-CG-SD
4	B	302	B3P	O2-C10-C8-N2
4	B	302	B3P	O2-C10-C8-C11

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SAM	5	0
2	B	301	SAM	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/298 (86%)	-0.03	2 (0%) 86 84	6, 13, 22, 27	0
1	B	265/298 (88%)	-0.12	4 (1%) 73 70	4, 9, 25, 32	0
All	All	522/596 (87%)	-0.08	6 (1%) 80 78	4, 11, 23, 32	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55[A]	HIS	3.9
1	B	266	ASP	3.7
1	B	2	SER	2.9
1	B	7	TRP	2.7
1	A	265	PRO	2.6
1	A	121	ARG	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](#)

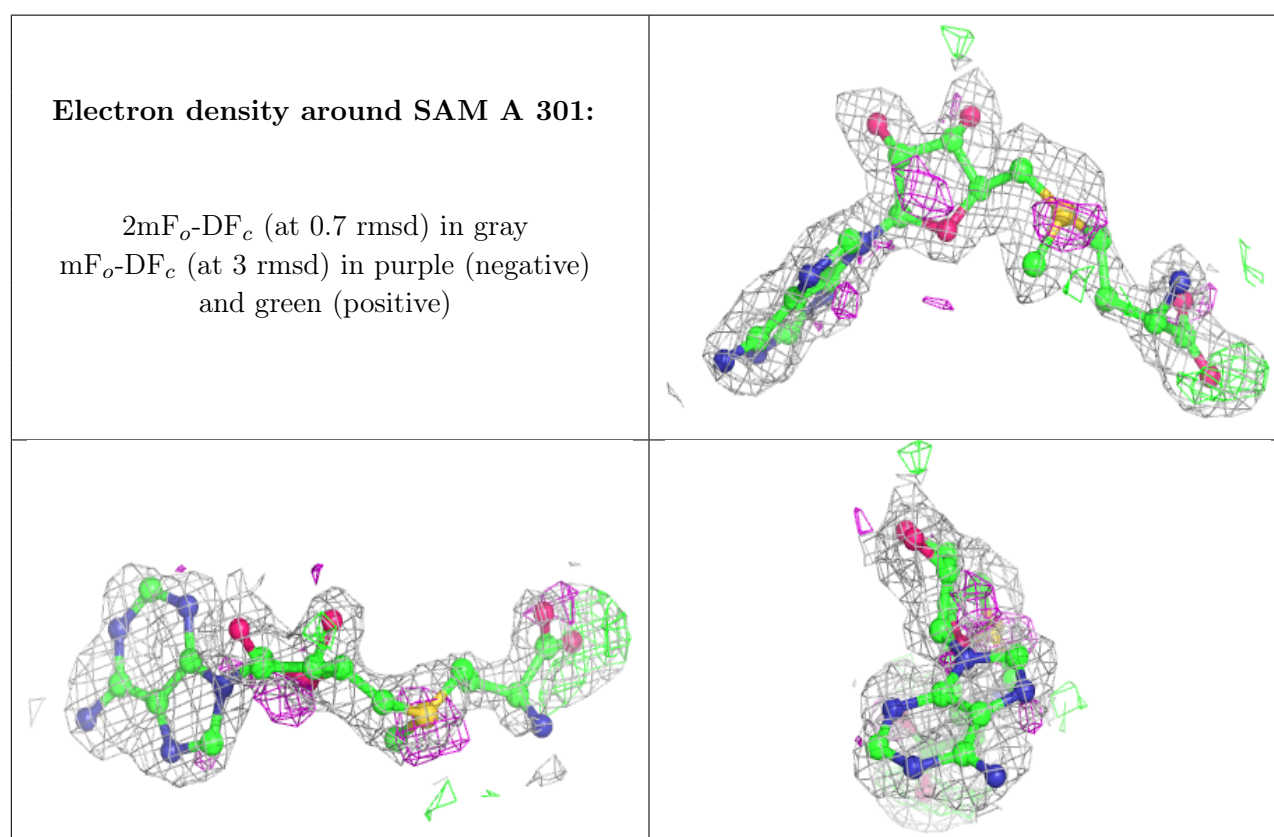
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SAM	A	301	27/27	0.77	0.22	19,29,39,45	0
4	B3P	B	302	19/19	0.88	0.16	11,23,39,41	0
2	SAM	B	301	27/27	0.92	0.12	13,18,30,42	0
3	BR	A	300	1/1	0.98	0.04	23,23,23,23	0
3	BR	B	299	1/1	0.99	0.06	13,13,13,13	0
3	BR	A	299	1/1	0.99	0.06	16,16,16,16	0

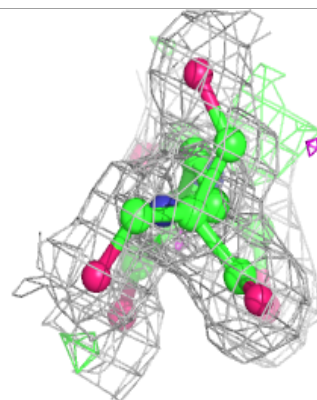
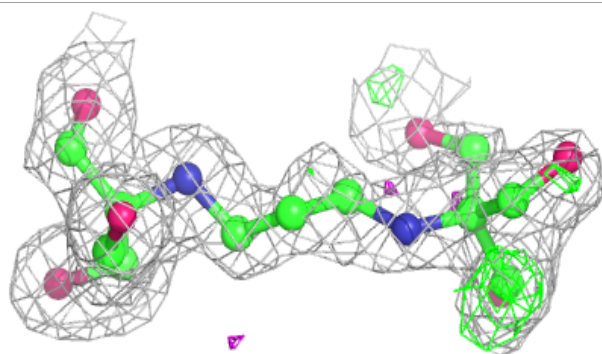
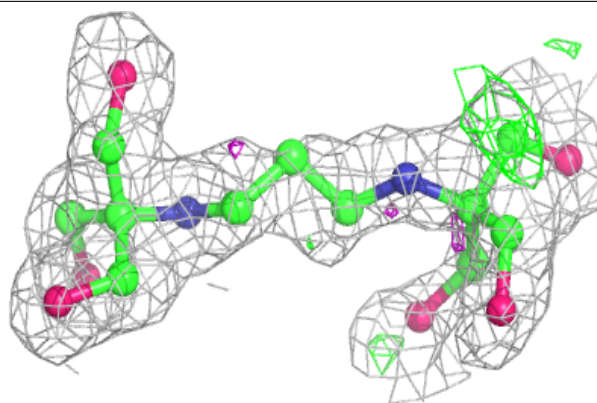
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



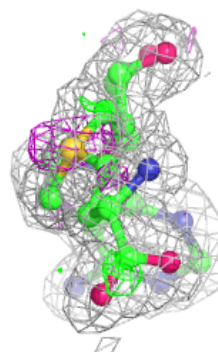
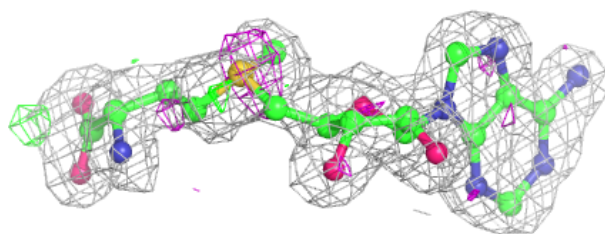
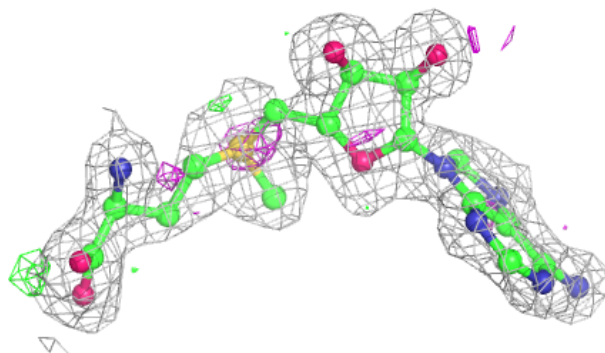


**Electron density around B3P B 302:**

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

**Electron density around SAM 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.