



## wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 01:50 PM EDT

PDB ID : 3JAY  
EMDB ID: : EMD-6378  
Title : Atomic model of transcribing cytoplasmic polyhedrosis virus  
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.  
Deposited on : 2015-07-06  
Resolution : 3.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

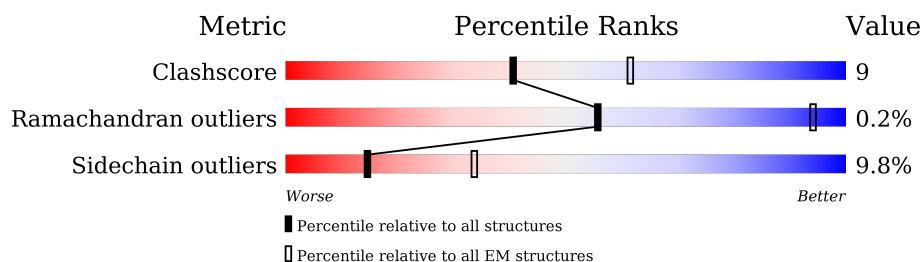
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32368 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

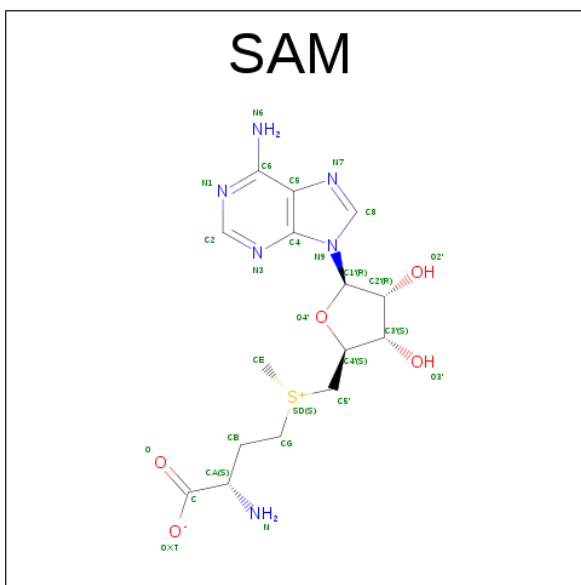
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1251	Total	C	N	O	S	0	0
			9857	6222	1713	1884	38		

- Molecule 3 is a protein called Viral structural protein 5.

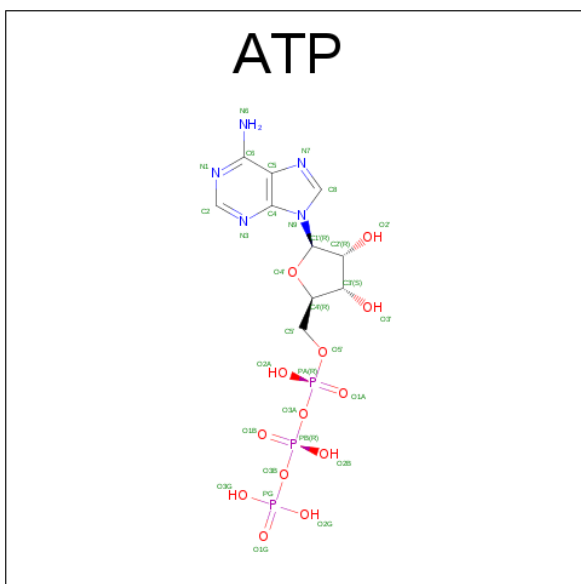
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 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).



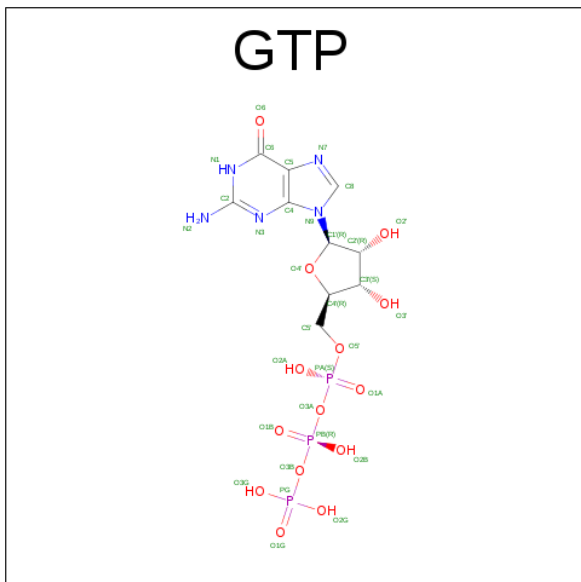
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 54	C 30	N 12	O 10	S 2	0
4	A	1	Total 54	C 30	N 12	O 10	S 2	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	32	10	5	14	3	0

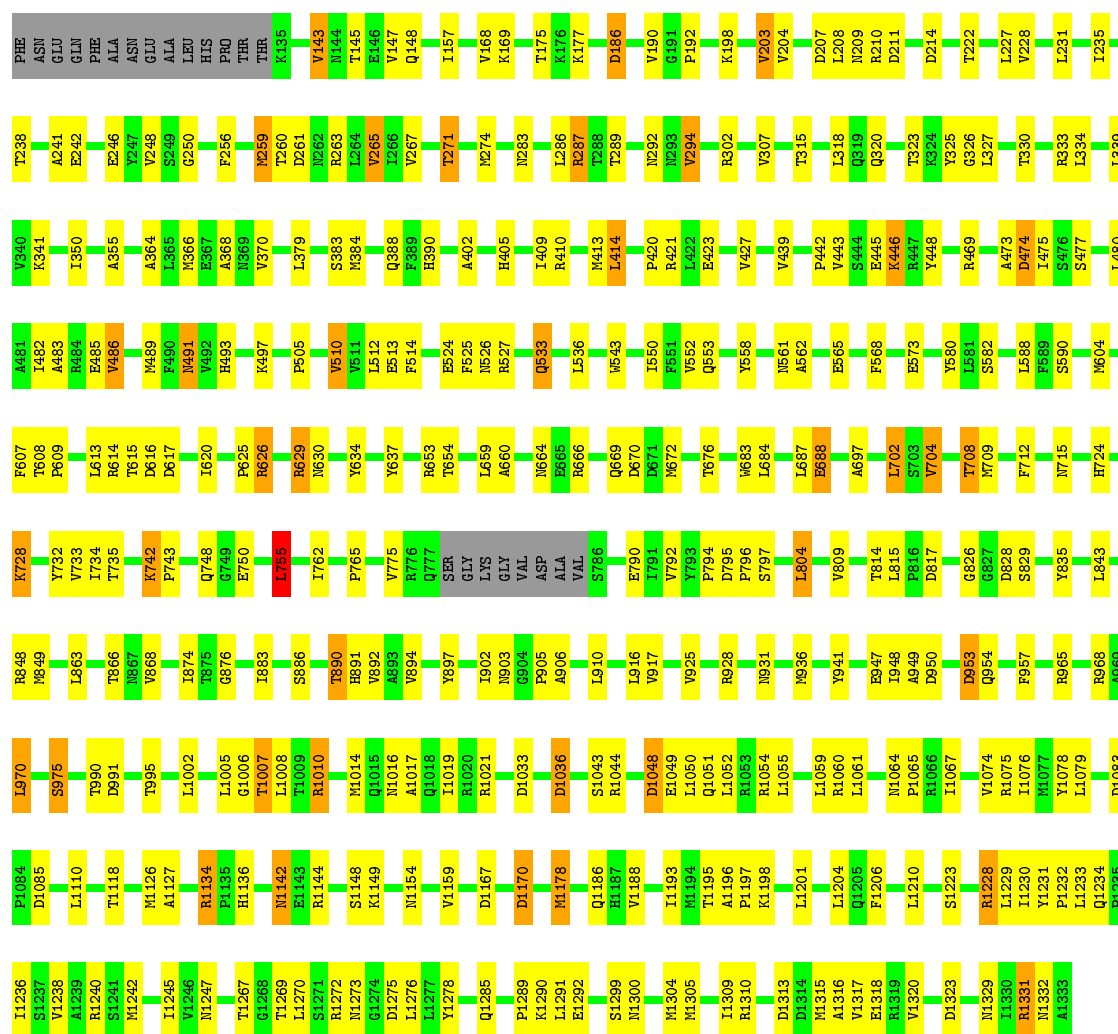
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

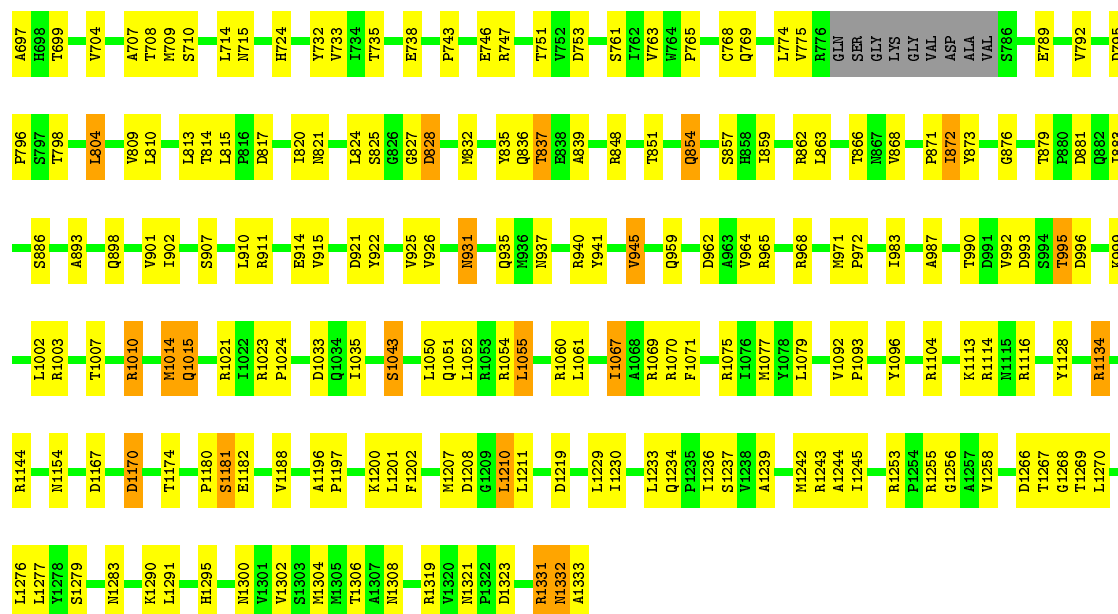
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	A	1	1	1	0



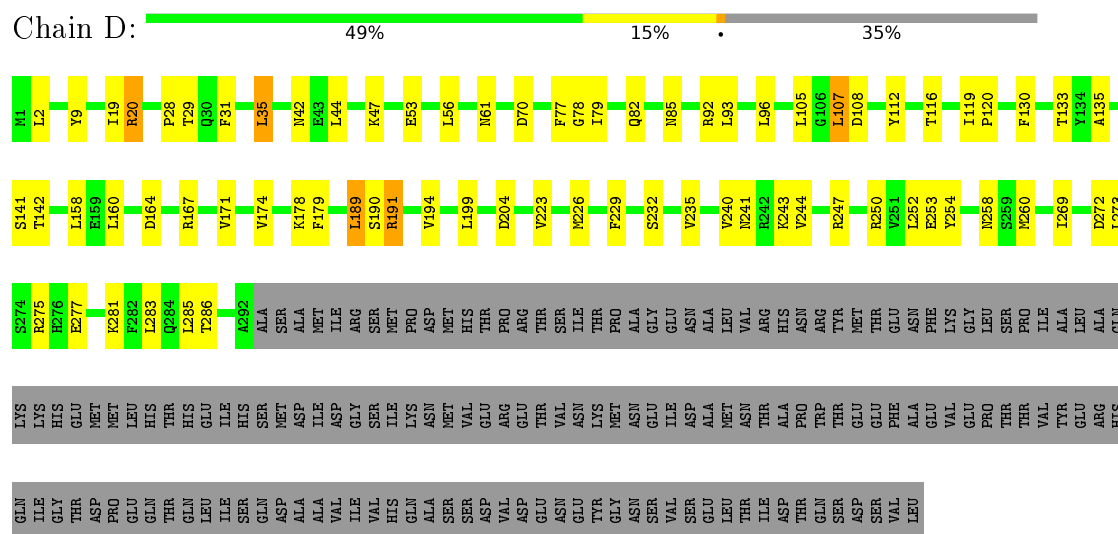
- Molecule 1: Structural protein VP3



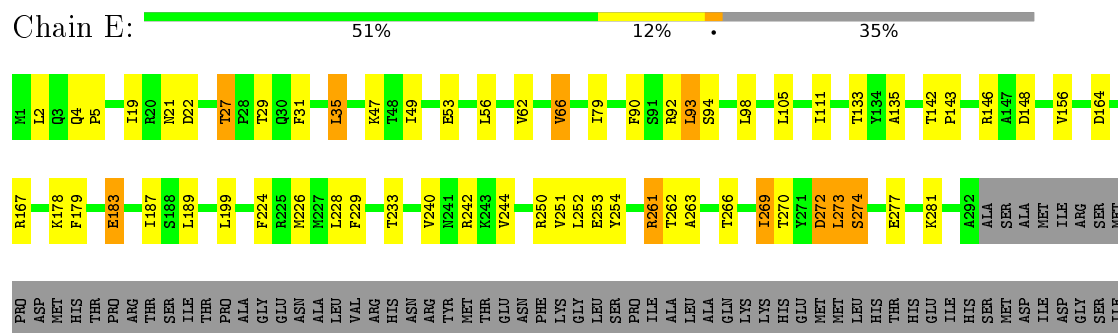




• Molecule 3: Viral structural protein 5



• Molecule 3: Viral structural protein 5





LYS	ASN	MET	VAL	GLU	ARG	GLU	THR	VAL	ASN	LYS	MET	ASN	GLU	ILE	ASP	ALA	MET	ASN	THR	ALA	PRO	TRP	THR	GLU	GLU	PHE	GLY	GLU	GLU	GLU	VAL	GLU	PRO	THR	THR	THR	VAL	TYR	GLU	GLU	ASP	THR	PRO	GLU	GLN	GLN	THR	GLN	LEU	ILE	LEU	SER	SER	GLN	ASP	ALA	ALA	VAL	VAL	ILE	ILE	VAL	VAL	TYR
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GLN	ALA	SER	SER	ASP	VAL	ASP	GLU	ASN	GLU	TYR	GLY	ASN	SER	VAL	SER	GLU	LEU	THR	ILE	ASP	THR	GLN	SER	ASP	SER	VAL	LEU
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41624	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 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: GTP, MG, ATP, SAM

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.28	0/8619	0.49	0/11737
2	B	0.33	0/9590	0.57	1/13056 (0.0%)
2	C	0.34	0/10058	0.55	0/13695
3	D	0.31	0/2327	0.53	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.32	0/32921	0.54	1/44814 (0.0%)

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	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	755	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	A	46	ARG	Sidechain
1	A	52	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	8434	0	8399	170	0
2	B	9397	0	9315	190	0
2	C	9857	0	9767	180	0
3	D	2281	0	2282	43	0
3	E	2281	0	2282	31	0
4	A	54	0	44	1	0
5	A	31	0	12	0	0
6	A	32	0	12	1	0
7	A	1	0	0	0	0
All	All	32368	0	32113	589	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 9.

The worst 5 of 589 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:52:ARG:NH2	1:A:52:ARG:HB2	1.72	1.02
1:A:43:ASN:OD1	1:A:46:ARG:HG2	1.72	0.89
1:A:41:THR:HG23	1:A:50:THR:HG23	1.56	0.88
2:C:383:SER:HB3	2:C:796:PRO:HG3	1.57	0.87
2:C:1134:ARG:NH2	2:C:1154:ASN:OD1	2.12	0.82

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 PDB entries followed by that with respect to all EM entries.

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	1055/1058 (100%)	1009 (96%)	45 (4%)	1 (0%)	56	90
2	B	1187/1333 (89%)	1129 (95%)	55 (5%)	3 (0%)	46	84
2	C	1247/1333 (94%)	1188 (95%)	55 (4%)	4 (0%)	46	84
3	D	290/448 (65%)	279 (96%)	10 (3%)	1 (0%)	46	84
3	E	290/448 (65%)	283 (98%)	7 (2%)	0	100	100
All	All	4069/4620 (88%)	3888 (96%)	172 (4%)	9 (0%)	56	88

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1136	HIS
2	C	769	GLN
2	B	790	GLU
2	B	1310	ARG
2	C	1014	MET

### 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 PDB entries followed by that with respect to all EM entries.

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	942/943 (100%)	853 (91%)	89 (9%)	11	39
2	B	1038/1153 (90%)	933 (90%)	105 (10%)	9	34
2	C	1090/1153 (94%)	978 (90%)	112 (10%)	9	33
3	D	240/379 (63%)	220 (92%)	20 (8%)	14	46
3	E	240/379 (63%)	217 (90%)	23 (10%)	10	38
All	All	3550/4007 (89%)	3201 (90%)	349 (10%)	14	36

5 of 349 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	975	SER
2	C	83	GLN
3	D	191	ARG

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Mol	Chain	Res	Type
2	B	1033	ASP
2	B	1193	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	576	ASN
2	B	724	HIS
2	C	1015	GLN
1	A	375	HIS
2	C	724	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z  > 2$
4	SAM	A	1101	-	23,29,29	1.03	2 (8%)	15,42,42	3.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SAM	A	1102	-	23,29,29	1.05	2 (8%)	15,42,42	2.99	1 (6%)
5	ATP	A	1103	-	26,33,33	0.92	1 (3%)	26,52,52	1.80	3 (11%)
6	GTP	A	1104	7	26,34,34	0.97	1 (3%)	29,54,54	1.62	5 (17%)

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
4	SAM	A	1101	-	-	0/8/33/33	0/3/3/3
4	SAM	A	1102	-	-	0/8/33/33	0/3/3/3
5	ATP	A	1103	-	-	0/18/38/38	0/3/3/3
6	GTP	A	1104	7	-	0/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N1	2.28	1.38	1.33
4	A	1102	SAM	C2-N1	2.38	1.38	1.33
5	A	1103	ATP	C5-C4	2.99	1.47	1.40
6	A	1104	GTP	C6-N1	3.16	1.38	1.33
4	A	1101	SAM	C2-N3	3.44	1.38	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	SAM	N3-C2-N1	-11.34	119.96	128.87
4	A	1102	SAM	N3-C2-N1	-11.21	120.07	128.87
5	A	1103	ATP	N3-C2-N1	-6.93	123.43	128.87
6	A	1104	GTP	N3-C2-N1	-5.30	120.34	127.56
6	A	1104	GTP	C5-C6-N1	-2.96	119.66	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1104	GTP	1	0

## 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.