



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:31 PM EDT

PDB ID : 3JB3
EMDB ID: : EMD-6377
Title : Atomic model of cytoplasmic polyhedrosis virus with SAM, GTP and ATP
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 3.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

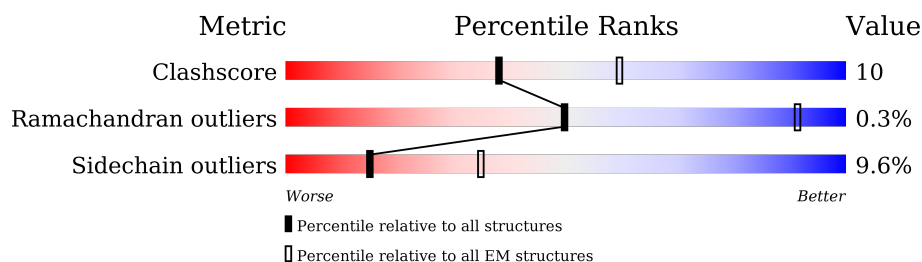
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	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 ≥ 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	70% 26% .
2	B	1333	63% 23% . 11%
2	C	1333	66% 24% . 6%
3	D	448	46% 17% . 35%
3	E	448	49% 15% . 35%

2 Entry composition

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		

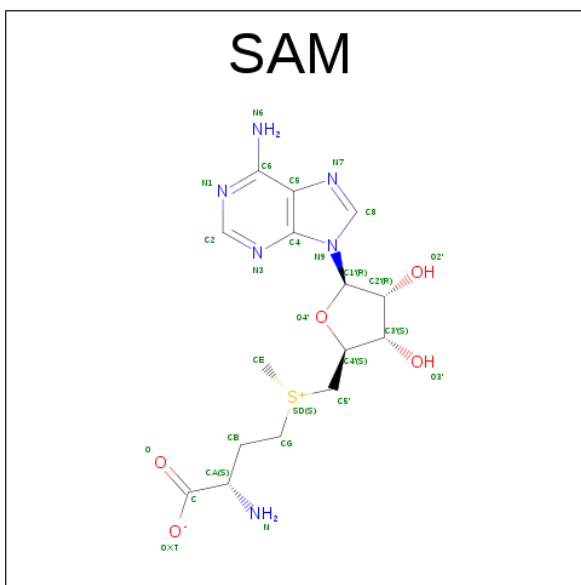
- Molecule 2 is a protein called Capsid protein VP1.

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.

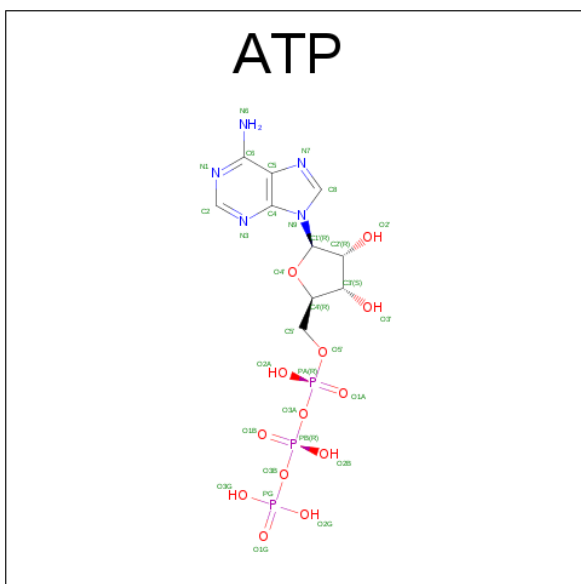
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



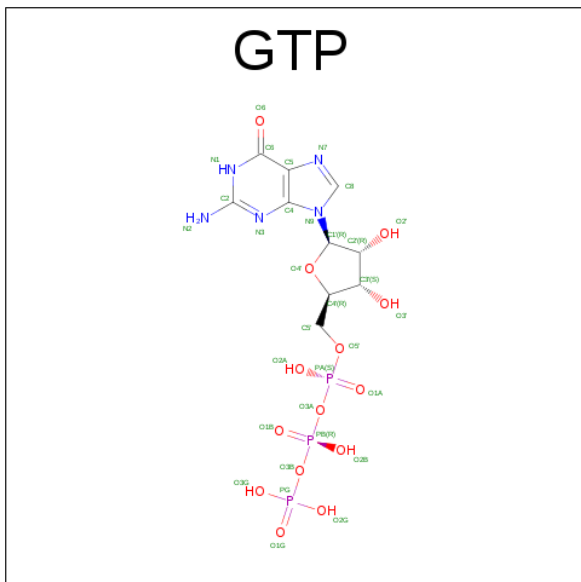
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 54	C 30	N 12	O 10	S 2	0
4	A	1	Total 54	C 30	N 12	O 10	S 2	0

- 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
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

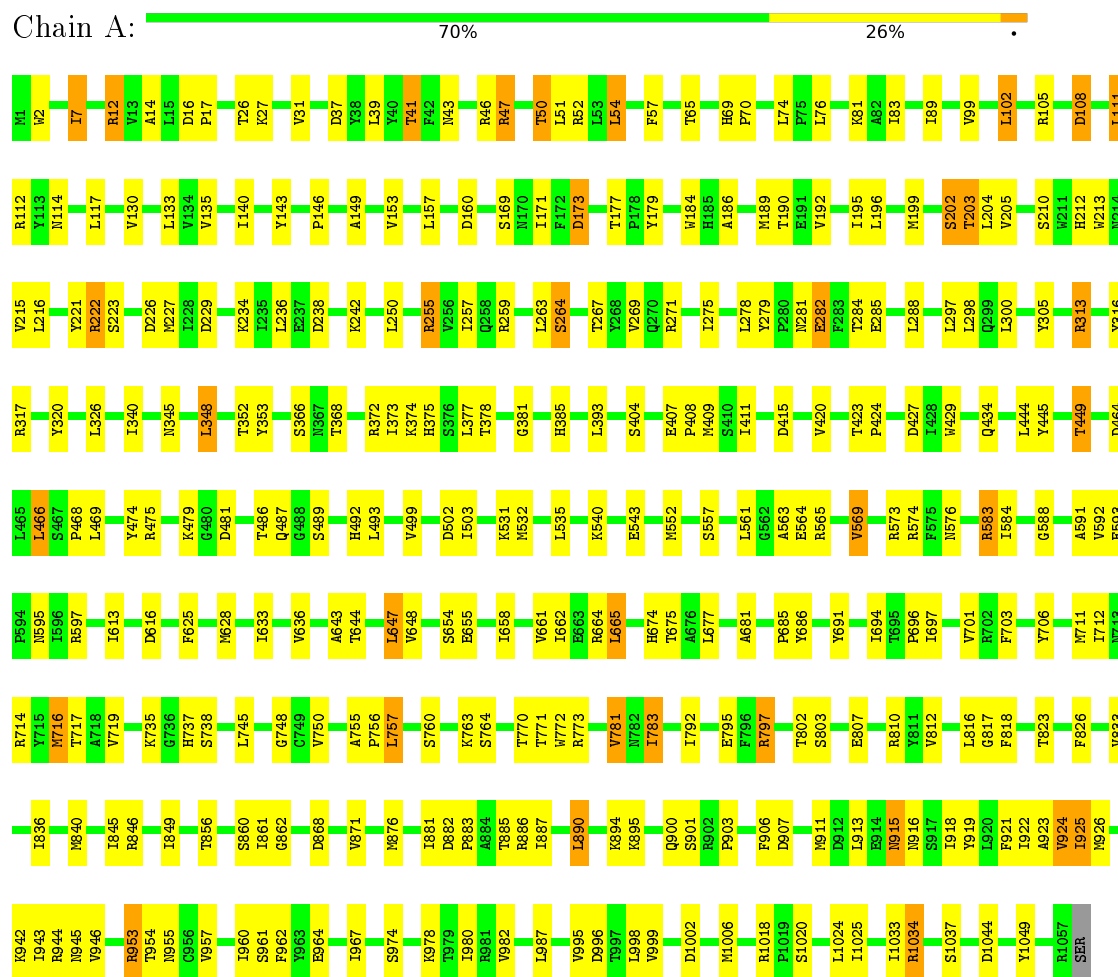
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

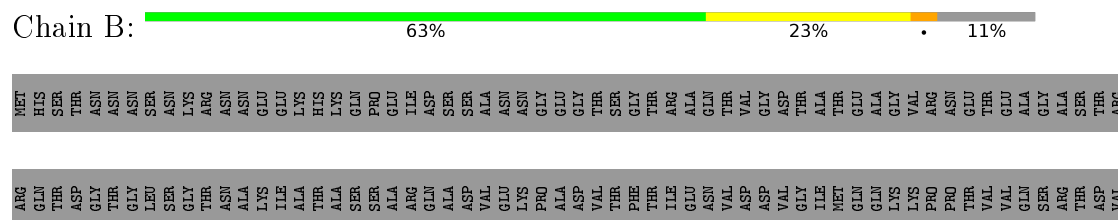
3 Residue-property plots

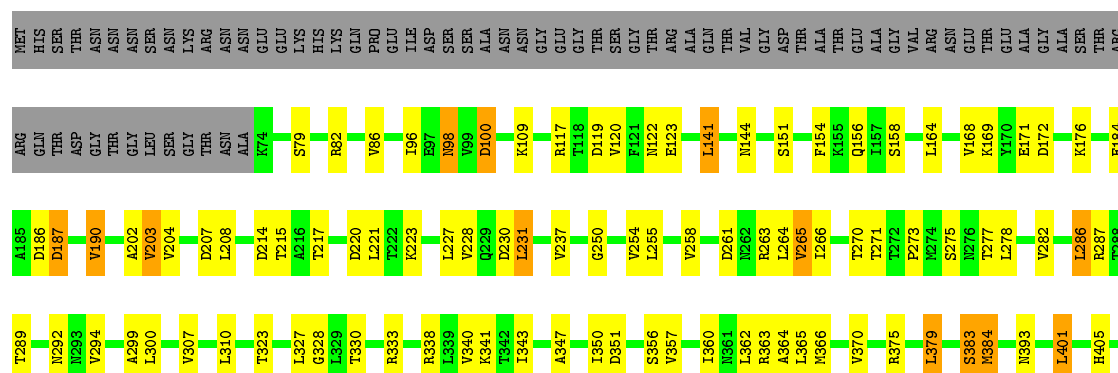
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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.

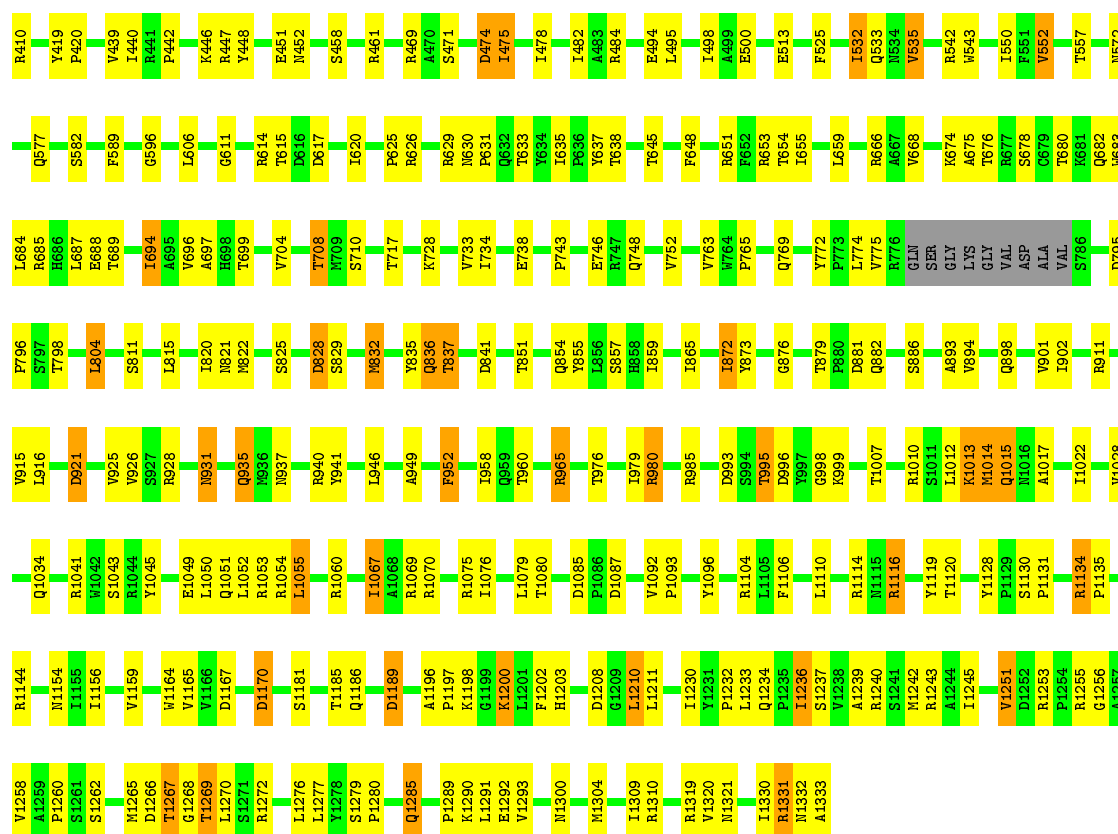
• Molecule 1: Structural protein VP3



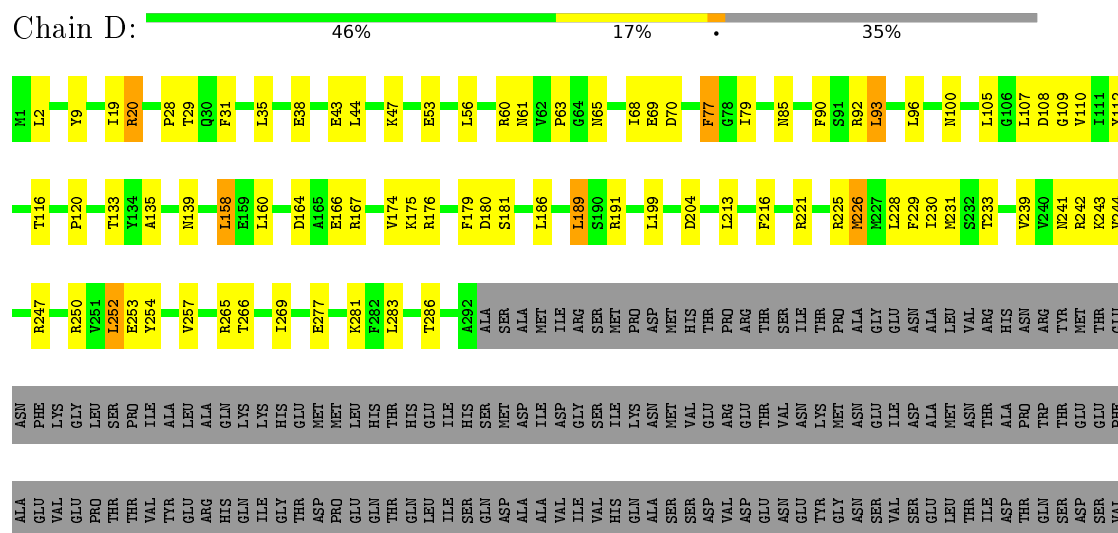
• Molecule 2: Capsid protein VP1







• Molecule 3: Viral structural protein 5



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• Molecule 3: Viral structural protein 5



	HIS	F282	L160	M1
GLN	THR	L283	T163	L2
THR	HIS	T286	D164	T6
LEU	ILE			
ILE	HIS	A292	R167	T10
SER	THR	ALA		
GLN	SER	ALA	P173	N21
GLN	ASP	MET	V174	D22
ALA	ALA	ILE	K175	
VAL	ASP	ILE		T27
ILE	GLY	ARG	K178	F28
VAL	SER	THR	F179	T29
HIS	ILE	MET	D180	Q30
GLN	LYS	PRO		
ALA	ASN	ASP	E183	L35
SER	MET	MET		
SER	VAL	HIS	L189	L44
ASP	GLU	THR		
VAL	ARG	PRO	L199	E53
ASP	GLU	ARG		
GLU	THR	THR	D204	L56
ASN	VAL	SER		
GLU	ASN	ILE	F224	V62
TYR	LYS	THR	R225	
GLY	MET	PRO	M226	V66
ASN	ASN	ALA	M227	V67
SER	GLU	GLY	L228	I68
VAL	ILE	GLU	F229	
SER	ASP	ASN		F90
GLU	ALA	ALA	T233	S91
LEU	MET	LEU	R92	R92
THR	ASN	VAL	N238	L93
ILE	THR	ARG	V239	
ALA	ALA	HIS	V240	L96
ASP	PRO	ASN		A97
THR	TRP	ARG	V244	L98
GLN	SER	TYR	T245	
ASP	GLU	MET	K246	T101
SER	GLU	THR	R247	
VAL	PHE	GLU	V248	L105
LEU	ALA	ASN	D249	
	GLU	PHE	R250	I111
	VAL	LYS	V251	
	GLU	GLY	L252	T116
	PRO	LEU	E253	
	THR	SER	Y254	D123
	THR	PRO		P124
	VAL	ILE	T262	
	TYR	ALA	A263	V127
	GLU	LEU		
	ARG	ALA	T266	F130
	HIS	GLN		
	GLN	LYS	T270	T133
	ILE	LYS	Z271	A135
	GLY	HIS	D272	
	THR	GLU	L273	T142
	ASP	MET	S274	P143
	PRO	MET		
	GLU	LEU	V284	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	40898	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	0.51	0/11737
2	B	0.34	0/9590	0.56	0/13056
2	C	0.34	0/10058	0.56	0/13695
3	D	0.32	0/2327	0.53	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.32	0/32921	0.54	0/44814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8398	175	0
2	B	9397	0	9315	194	0
2	C	9857	0	9767	193	0
3	D	2281	0	2282	47	0
3	E	2281	0	2282	32	0
4	A	54	0	44	3	0
5	A	31	0	12	3	0
6	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
All	All	32368	0	32112	624	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 10.

The worst 5 of 624 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:267:THR:HG22	1:A:271:ARG:HE	1.41	0.83
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.64	0.79
1:A:305:TYR:O	1:A:317:ARG:NH1	2.16	0.78
2:B:1144:ARG:NH1	2:B:1170:ASP:OD1	2.17	0.78
5:A:1103:ATP:H8	5:A:1103:ATP:H5'1	1.50	0.77

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 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%)	1002 (95%)	53 (5%)	0	100	100
2	B	1187/1333 (89%)	1126 (95%)	58 (5%)	3 (0%)	46	80
2	C	1247/1333 (94%)	1191 (96%)	49 (4%)	7 (1%)	30	68
3	D	290/448 (65%)	282 (97%)	6 (2%)	2 (1%)	26	65
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	46	80
All	All	4069/4620 (88%)	3883 (95%)	173 (4%)	13 (0%)	50	80

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	769	GLN
2	C	1251	VAL
3	D	61	ASN
2	B	1310	ARG
2	C	340	VAL

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%)	850 (90%)	92 (10%)	10	36
2	B	1038/1153 (90%)	946 (91%)	92 (9%)	12	42
2	C	1090/1153 (94%)	974 (89%)	116 (11%)	8	31
3	D	240/379 (63%)	221 (92%)	19 (8%)	15	49
3	E	240/379 (63%)	218 (91%)	22 (9%)	11	40
All	All	3550/4007 (89%)	3209 (90%)	341 (10%)	15	37

5 of 341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	991	ASP
2	C	120	VAL
3	D	226	MET
2	B	1041	ARG
2	B	1198	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	430	ASN
3	D	85	ASN
2	B	1138	HIS
1	A	576	ASN
2	C	931	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.05	2 (8%)	15,42,42	3.05	2 (13%)
4	SAM	A	1102	-	23,29,29	1.07	2 (8%)	15,42,42	2.98	1 (6%)
5	ATP	A	1103	-	26,33,33	0.93	1 (3%)	26,52,52	1.71	5 (19%)
6	GTP	A	1104	7	26,34,34	0.93	1 (3%)	29,54,54	1.59	4 (13%)

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	2.40	1.38	1.33
4	A	1102	SAM	C2-N1	2.42	1.38	1.33
5	A	1103	ATP	C5-C4	3.01	1.47	1.40
6	A	1104	GTP	C6-N1	3.04	1.38	1.33
4	A	1102	SAM	C2-N3	3.50	1.38	1.32

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	SAM	N3-C2-N1	-11.27	120.02	128.87
4	A	1102	SAM	N3-C2-N1	-11.00	120.23	128.87
5	A	1103	ATP	N3-C2-N1	-6.11	124.07	128.87
6	A	1104	GTP	N3-C2-N1	-5.42	120.18	127.56
6	A	1104	GTP	C5-C6-N1	-2.93	119.69	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	2	0
4	A	1102	SAM	1	0
5	A	1103	ATP	3	0
6	A	1104	GTP	3	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.