Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:48 PM GMT

PDB ID	:	1CKN
Title	:	STRUCTURE OF GUANYLYLATED MRNA CAPPING ENZYME COMPLEXED WITH GTP
Authors	:	Hakansson, K.; Doherty, A.J.; Wigley, D.B.
Deposited on	:	1997-04-20
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

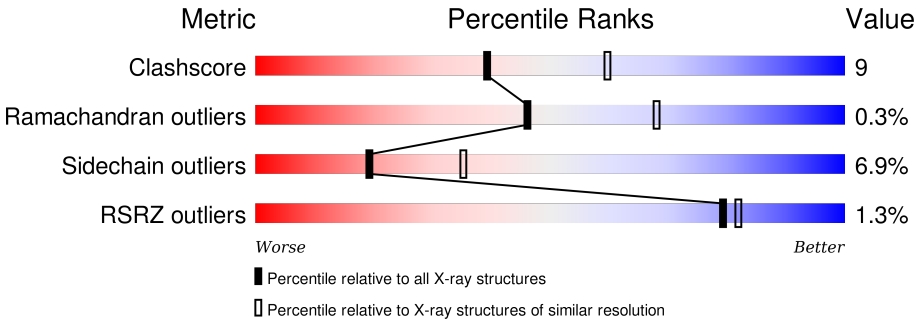
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower 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 <=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	330	2% 69% 24%
2	B	330	% 63% 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5525 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 MRNA CAPPING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2561	1657	429	463	12			

- Molecule 2 is a protein called MRNA CAPPING ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	317	Total	C	N	O	P	S	0	0	0
			2584	1667	434	470	1	12			

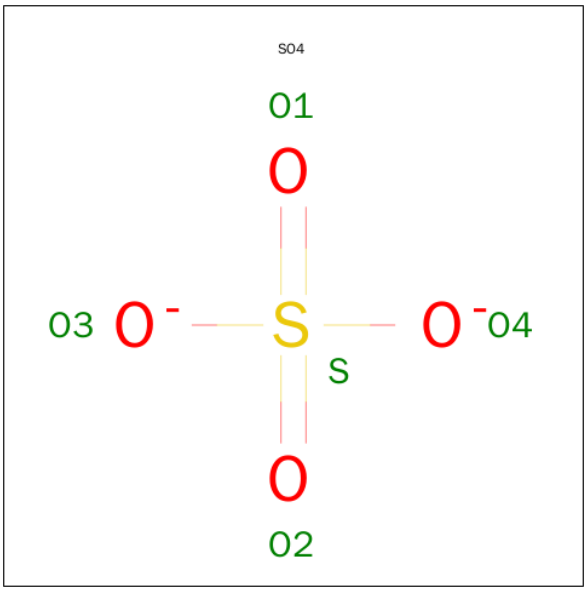
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	GPL	LYS	CONFLICT	UNP Q84424

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

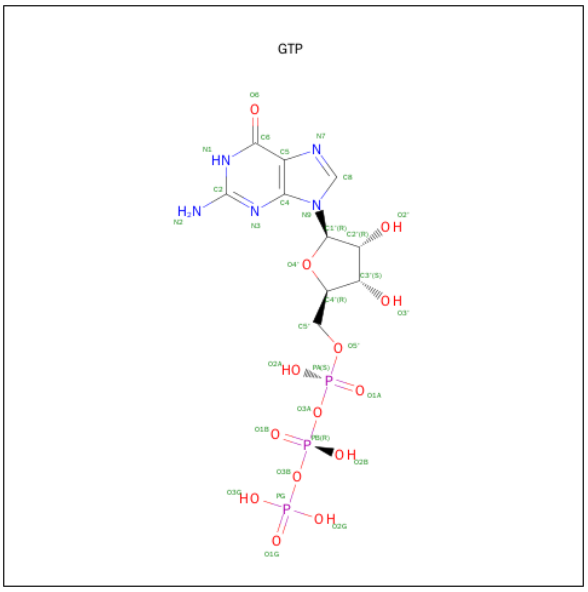
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0

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



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

- Molecule 6 is water.

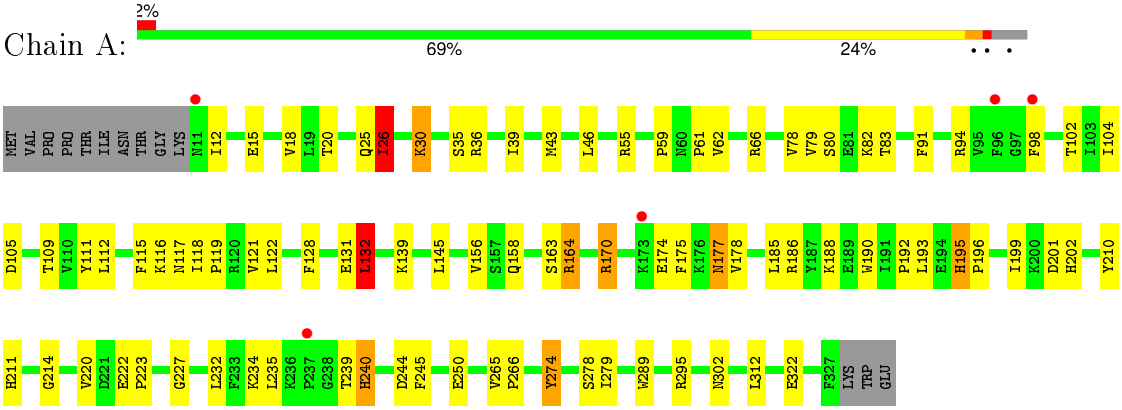
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	165	Total O 165 165	0	0
6	B	177	Total O 177 177	0	0

3 Residue-property plots (i)

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 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.

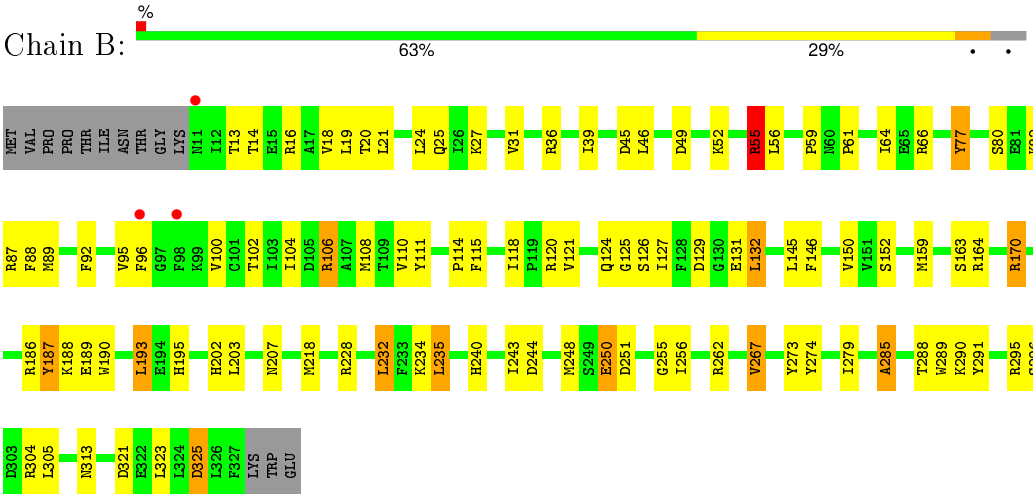
- Molecule 1: MRNA CAPPING ENZYME

Chain A:



- Molecule 2: MRNA CAPPING ENZYME

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	94.91Å 212.95Å 105.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 14.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (10.00-2.50) 95.4 (14.99-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.224 , 0.299 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 81.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 36093 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5525	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GPL, GTP, MN, SO4

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	0.78	0/2616	1.40	21/3530 (0.6%)
2	B	0.78	0/2606	1.45	33/3516 (0.9%)
All	All	0.78	0/5222	1.43	54/7046 (0.8%)

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
2	B	0	6
All	All	0	11

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ARG	NE-CZ-NH2	-10.63	114.98	120.30
2	B	289	TRP	CD1-CG-CD2	9.64	114.02	106.30
2	B	289	TRP	CE2-CD2-CG	-9.28	99.88	107.30
1	A	289	TRP	CD1-CG-CD2	9.22	113.67	106.30
1	A	164	ARG	NE-CZ-NH2	-8.76	115.92	120.30
2	B	66	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	B	164	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	164	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	289	TRP	CE2-CD2-CG	-7.91	100.97	107.30
2	B	164	ARG	NE-CZ-NH2	-7.83	116.39	120.30
2	B	106	ARG	NE-CZ-NH2	-7.82	116.39	120.30
2	B	106	ARG	NE-CZ-NH1	7.77	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	87	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	186	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	B	190	TRP	CD1-CG-CD2	7.23	112.08	106.30
1	A	170	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	B	190	TRP	CE2-CD2-CG	-7.05	101.66	107.30
2	B	87	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	304	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	190	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	190	TRP	CD1-CG-CD2	6.57	111.56	106.30
2	B	120	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	B	170	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	B	55	ARG	CB-CA-C	-6.28	97.83	110.40
2	B	289	TRP	CG-CD2-CE3	6.17	139.45	133.90
2	B	267	VAL	N-CA-CB	-6.13	98.01	111.50
2	B	150	VAL	CG1-CB-CG2	-6.11	101.12	110.90
2	B	187	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	B	55	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	B	289	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	A	94	ARG	NE-CZ-NH2	-5.91	117.34	120.30
2	B	228	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	240	HIS	CA-CB-CG	5.70	123.30	113.60
1	A	210	TYR	CB-CG-CD2	-5.70	117.58	121.00
2	B	55	ARG	CA-CB-CG	5.57	125.66	113.40
2	B	289	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	A	91	PHE	CB-CG-CD2	-5.51	116.94	120.80
2	B	218	MET	CG-SD-CE	-5.50	91.40	100.20
1	A	289	TRP	CG-CD1-NE1	-5.46	104.64	110.10
2	B	186	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	36	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	295	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	274	TYR	CB-CG-CD2	-5.39	117.77	121.00
2	B	285	ALA	CB-CA-C	-5.33	102.10	110.10
1	A	132	LEU	CA-CB-CG	5.32	127.54	115.30
2	B	66	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	B	251	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	26	ILE	CB-CA-C	-5.17	101.27	111.60
1	A	177	ASN	CB-CA-C	-5.16	100.08	110.40
2	B	304	ARG	CA-CB-CG	5.09	124.60	113.40
1	A	105	ASP	CA-CB-CG	5.09	124.59	113.40
2	B	295	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	66	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	B	299	ASN	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	TYR	Sidechain
1	A	170	ARG	Sidechain
1	A	274	TYR	Sidechain
1	A	295	ARG	Sidechain
1	A	98	PHE	Sidechain
2	B	106	ARG	Sidechain
2	B	111	TYR	Sidechain
2	B	187	TYR	Sidechain
2	B	273	TYR	Sidechain
2	B	274	TYR	Sidechain
2	B	77	TYR	Sidechain

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	2561	0	2607	41	0
2	B	2584	0	2617	54	0
3	B	1	0	0	0	0
4	B	5	0	0	0	0
5	A	32	0	12	5	0
6	A	165	0	0	7	0
6	B	177	0	0	4	0
All	All	5525	0	5236	93	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.

All (93) 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:26:ILE:HD11	1:A:132:LEU:HD11	1.61	0.81
1:A:156:VAL:HG12	1:A:164:ARG:HG2	1.71	0.73
2:B:83:THR:HB	2:B:131:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:MET:CE	2:B:163:SER:HB3	2.26	0.66
1:A:158:GLN:HA	1:A:223:PRO:HB3	1.81	0.63
2:B:285:ALA:HB2	2:B:290:LYS:HD2	1.80	0.62
2:B:21:LEU:HD21	2:B:86:ILE:HG13	1.82	0.61
2:B:104:ILE:HG12	2:B:110:VAL:HG22	1.82	0.61
1:A:39:ILE:HD13	1:A:102:THR:HG21	1.82	0.61
2:B:202:HIS:HB2	6:B:1105:HOH:O	2.00	0.61
1:A:20:THR:HG23	1:A:25:GLN:HG2	1.84	0.60
1:A:61:PRO:HG2	5:A:899:GTP:H5'	1.82	0.60
2:B:131:GLU:HG2	2:B:146:PHE:HZ	1.68	0.58
2:B:248:MET:SD	2:B:255:GLY:HA3	2.43	0.58
2:B:77:TYR:HB2	2:B:193:LEU:HD12	1.85	0.58
2:B:100:VAL:HG12	2:B:102:THR:HG23	1.87	0.57
1:A:79:VAL:HG11	1:A:199:ILE:HD13	1.87	0.56
1:A:156:VAL:HG11	1:A:164:ARG:HA	1.87	0.56
2:B:145:LEU:O	2:B:188:LYS:HB2	2.06	0.55
1:A:214:GLY:HA3	1:A:235:LEU:O	2.07	0.55
2:B:321:ASP:O	2:B:325:ASP:HB2	2.06	0.55
1:A:18:VAL:HA	1:A:26:ILE:O	2.07	0.55
2:B:89:MET:HE1	2:B:129:ASP:HB2	1.88	0.55
1:A:12:ILE:HG23	1:A:35:SER:HB3	1.89	0.54
1:A:163:SER:HA	6:A:1026:HOH:O	2.08	0.54
2:B:159:MET:HE3	2:B:163:SER:HB3	1.88	0.54
2:B:159:MET:HE2	2:B:163:SER:HB3	1.88	0.54
2:B:82:GPL:HE2	2:B:234:LYS:HD2	1.89	0.54
2:B:95:VAL:HG12	2:B:96:PHE:CD2	2.43	0.54
2:B:61:PRO:HG3	2:B:232:LEU:HD13	1.88	0.54
1:A:82:LYS:HE3	5:A:899:GTP:H5"	1.90	0.53
2:B:121:VAL:HG22	2:B:152:SER:HB3	1.91	0.53
1:A:177:ASN:HD21	1:A:185:LEU:H	1.55	0.53
2:B:240:HIS:NE2	2:B:290:LYS:HE2	2.24	0.53
1:A:59:PRO:HA	1:A:227:GLY:O	2.09	0.52
2:B:115:PHE:HB2	2:B:118:ILE:CD1	2.40	0.52
2:B:121:VAL:HG23	2:B:124:GLN:OE1	2.09	0.52
1:A:119:PRO:HB2	1:A:122:LEU:HD23	1.92	0.51
2:B:64:ILE:HG21	2:B:235:LEU:HG	1.91	0.51
1:A:202:HIS:HB2	6:A:1012:HOH:O	2.11	0.50
2:B:244:ASP:H	2:B:302:ASN:ND2	2.09	0.50
1:A:15:GLU:O	1:A:30:LYS:N	2.44	0.50
1:A:188:LYS:NZ	5:A:899:GTP:O6	2.44	0.50
2:B:313:ASN:HA	6:B:1023:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:ND1	2:B:291:TYR:HB3	2.27	0.49
1:A:115:PHE:HB2	1:A:118:ILE:HG12	1.95	0.49
1:A:83:THR:HB	1:A:131:GLU:HG2	1.96	0.48
2:B:115:PHE:HE2	2:B:183:ALA:O	1.97	0.47
1:A:78:VAL:HG13	1:A:220:VAL:HG23	1.95	0.47
2:B:20:THR:HA	2:B:24:LEU:O	2.14	0.47
2:B:46:LEU:HD23	2:B:127:ILE:HG13	1.96	0.47
2:B:80:SER:OG	2:B:188:LYS:HE3	2.15	0.47
1:A:25:GLN:HG3	2:B:18:VAL:HG21	1.97	0.47
1:A:116:LYS:HD3	1:A:178:VAL:HG11	1.97	0.47
2:B:19:LEU:O	2:B:25:GLN:HA	2.15	0.46
1:A:61:PRO:CG	5:A:899:GTP:H5'	2.45	0.46
1:A:240:HIS:ND1	6:A:900:HOH:O	2.35	0.46
1:A:117:ASN:O	1:A:175:PHE:HD1	1.98	0.46
2:B:59:PRO:HB2	2:B:232:LEU:HD12	1.97	0.46
2:B:243:ILE:HA	2:B:302:ASN:HD22	1.79	0.46
1:A:30:LYS:HD2	1:A:109:THR:HG23	1.97	0.46
1:A:192:PRO:HB3	6:A:931:HOH:O	2.15	0.46
2:B:170:ARG:O	2:B:173:LYS:HG2	2.17	0.45
1:A:244:ASP:H	1:A:302:ASN:ND2	2.14	0.45
1:A:234:LYS:HD2	5:A:899:GTP:O2A	2.17	0.44
2:B:195:HIS:CE1	6:B:1107:HOH:O	2.70	0.44
2:B:92:PHE:HE2	2:B:118:ILE:HD13	1.83	0.44
2:B:14:THR:HG22	2:B:31:VAL:HA	1.99	0.44
1:A:211:HIS:HD2	6:A:1018:HOH:O	2.01	0.44
2:B:56:LEU:HD22	2:B:89:MET:HB2	2.01	0.43
2:B:115:PHE:CD1	2:B:118:ILE:HD11	2.53	0.43
2:B:85:GLY:HA3	2:B:132:LEU:O	2.19	0.43
2:B:88:PHE:CD2	2:B:132:LEU:HB2	2.54	0.43
1:A:128:PHE:HB3	1:A:145:LEU:HD22	2.01	0.42
1:A:195:HIS:CE1	6:A:1063:HOH:O	2.72	0.42
2:B:89:MET:CE	2:B:127:ILE:HG22	2.49	0.42
2:B:114:PRO:HD2	2:B:182:PRO:HG3	2.02	0.42
2:B:290:LYS:NZ	6:B:1174:HOH:O	2.53	0.42
2:B:92:PHE:CE2	2:B:118:ILE:HD13	2.53	0.42
2:B:279:ILE:N	2:B:279:ILE:HD12	2.35	0.41
2:B:49:ASP:OD2	2:B:55:ARG:HD2	2.19	0.41
2:B:285:ALA:CB	2:B:290:LYS:HD2	2.49	0.41
1:A:164:ARG:NH2	1:A:222:GLU:O	2.53	0.41
2:B:92:PHE:HD1	2:B:126:SER:HB2	1.86	0.41
2:B:131:GLU:HG2	2:B:146:PHE:CZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HA	1:A:199:ILE:HD12	2.02	0.41
1:A:43:MET:SD	1:A:104:ILE:HD12	2.60	0.41
2:B:31:VAL:HG11	2:B:39:ILE:HD12	2.01	0.40
2:B:36:ARG:NH1	2:B:108:MET:O	2.54	0.40
1:A:278:SER:HB3	6:A:930:HOH:O	2.21	0.40
1:A:245:PHE:O	1:A:279:ILE:HA	2.22	0.40
2:B:203:LEU:O	2:B:207:ASN:ND2	2.50	0.40
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.95	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	315/330 (96%)	298 (95%)	17 (5%)	0	100	100
2	B	314/330 (95%)	297 (95%)	15 (5%)	2 (1%)	30	50
All	All	629/660 (95%)	595 (95%)	32 (5%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	GLU
2	B	125	GLY

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	285/297 (96%)	266 (93%)	19 (7%)	20 37
2	B	284/296 (96%)	264 (93%)	20 (7%)	19 34
All	All	569/593 (96%)	530 (93%)	39 (7%)	19 35

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	30	LYS
1	A	46	LEU
1	A	55	ARG
1	A	62	VAL
1	A	80	SER
1	A	112	LEU
1	A	121	VAL
1	A	132	LEU
1	A	139	LYS
1	A	174	GLU
1	A	193	LEU
1	A	195	HIS
1	A	201	ASP
1	A	232	LEU
1	A	239	THR
1	A	250	GLU
1	A	312	LEU
1	A	322	GLU
2	B	13	THR
2	B	16	ARG
2	B	27	LYS
2	B	45	ASP
2	B	52	LYS
2	B	55	ARG
2	B	132	LEU
2	B	189	GLU
2	B	193	LEU
2	B	232	LEU
2	B	235	LEU
2	B	250	GLU
2	B	256	ILE
2	B	262	ARG
2	B	267	VAL

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Mol	Chain	Res	Type
2	B	288	THR
2	B	296	SER
2	B	305	LEU
2	B	323	LEU
2	B	325	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	60	ASN
1	A	177	ASN
1	A	302	ASN
1	A	313	ASN
2	B	25	GLN
2	B	51	HIS
2	B	302	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	GPL	B	82	3,2	28,34,35	1.84	8 (28%)	30,49,51	2.80	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
2	GPL	B	82	3,2	-	1/14/37/39	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	GPL	P-O2P	-3.11	1.48	1.56
2	B	82	GPL	C5-C4	-2.35	1.35	1.40
2	B	82	GPL	C8-N7	-2.32	1.30	1.34
2	B	82	GPL	P-NZ	2.26	1.63	1.61
2	B	82	GPL	C2-N1	2.39	1.39	1.35
2	B	82	GPL	O4'-C1'	2.92	1.44	1.41
2	B	82	GPL	C6-N1	4.24	1.41	1.33
2	B	82	GPL	P-O1P	4.36	1.51	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	82	GPL	C5-C6-N1	-8.54	111.91	123.59
2	B	82	GPL	P-NZ-CE	-7.04	111.40	124.09
2	B	82	GPL	N3-C2-N1	-3.50	122.12	127.44
2	B	82	GPL	C4'-O4'-C1'	-3.16	106.24	109.72
2	B	82	GPL	CD-CG-CB	-2.01	106.53	113.66
2	B	82	GPL	O5'-C5'-C4'	2.54	118.49	109.12
2	B	82	GPL	O4'-C4'-C5'	2.81	119.39	109.32
2	B	82	GPL	O2P-P-O1P	2.88	116.02	110.00
2	B	82	GPL	O4'-C1'-N9	3.48	115.39	108.10
2	B	82	GPL	C6-N1-C2	6.19	124.53	115.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	82	GPL	P-O5'-C5'-C4'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	82	GPL	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	GTP	A	899	-	25,34,34	1.72	5 (20%)	34,54,54	2.33	6 (17%)
4	SO4	B	1000	-	4,4,4	0.86	0	6,6,6	0.45	0

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
5	GTP	A	899	-	-	0/18/38/38	0/3/3/3
4	SO4	B	1000	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	899	GTP	PA-O2A	-2.82	1.42	1.54
5	A	899	GTP	PG-O3G	-2.18	1.46	1.54
5	A	899	GTP	C8-N7	-2.03	1.30	1.34
5	A	899	GTP	O4'-C1'	4.11	1.46	1.41
5	A	899	GTP	C6-N1	4.22	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	899	GTP	C5-C6-N1	-8.72	111.66	123.59
5	A	899	GTP	N3-C2-N1	-3.71	121.80	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	899	GTP	C4'-O4'-C1'	-2.76	106.68	109.72
5	A	899	GTP	O3G-PG-O2G	2.12	115.47	107.38
5	A	899	GTP	O5'-C5'-C4'	2.19	117.21	109.12
5	A	899	GTP	C6-N1-C2	7.51	126.37	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	899	GTP	5	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	317/330 (96%)	-0.55	5 (1%)	74	78	8, 25, 55, 89	0
2	B	316/330 (95%)	-0.58	3 (0%)	85	88	7, 25, 56, 93	0
All	All	633/660 (95%)	-0.57	8 (1%)	79	82	7, 25, 55, 93	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	PHE	3.3
1	A	11	ASN	2.8
1	A	98	PHE	2.4
1	A	237	PRO	2.3
2	B	96	PHE	2.3
1	A	173	LYS	2.3
2	B	11	ASN	2.3
1	A	96	PHE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	GPL	B	82	32/33	0.97	0.09	-	4,16,25,31	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	GTP	A	899	32/32	0.92	0.14	0.72	15,36,130,135	0
4	SO4	B	1000	5/5	0.97	0.13	0.35	35,48,57,65	0
3	MN	B	1001	1/1	0.84	0.12	-	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.