



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:58 PM GMT

PDB ID : 4NCN
Title : Crystal structure of eukaryotic translation initiation factor eIF5B (517-858)
from Chaetomium thermophilum in complex with GTP
Authors : Kuhle, B.; Ficner, R.
Deposited on : 2013-10-24
Resolution : 1.87 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

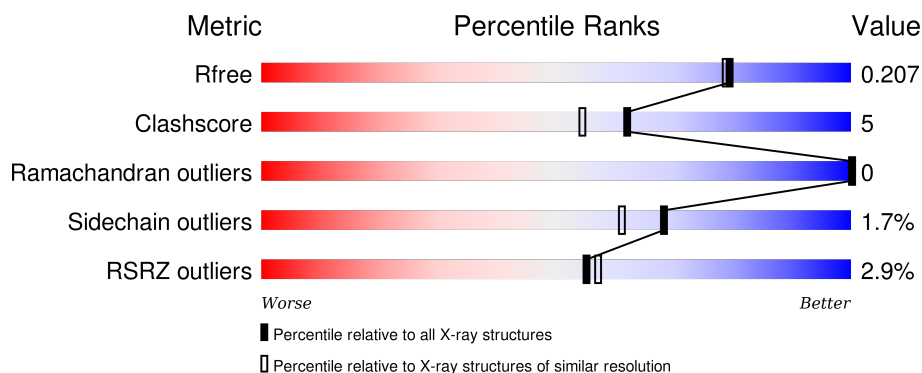
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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 $\leq 5\%$. 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	457	<div> <div>4%</div> <div>68%</div> <div>7%</div> <div>25%</div> </div>
1	B	457	<div> <div>65%</div> <div>10%</div> <div>25%</div> </div>

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
5	GOL	A	1004	-	-	-	X
5	GOL	A	1005	-	-	-	X
5	GOL	B	1005	-	-	-	X
5	GOL	B	1006	-	-	X	X
5	GOL	B	1007	-	-	-	X
5	GOL	B	1008	-	-	-	X
6	ACY	B	1004	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6087 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 Eukaryotic translation initiation factor 5B-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	4	0
			2724	1720	481	513	10			
1	B	345	Total	C	N	O	S	0	4	0
			2725	1721	479	514	11			

There are 54 discrepancies between the modelled and reference sequences:

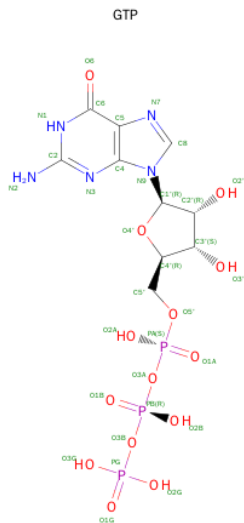
Chain	Residue	Modelled	Actual	Comment	Reference
A	514	SER	-	EXPRESSION TAG	UNP G0S8G9
A	515	HIS	-	EXPRESSION TAG	UNP G0S8G9
A	516	MET	-	EXPRESSION TAG	UNP G0S8G9
A	576	VAL	-	SEE REMARK 999	UNP G0S8G9
A	577	VAL	-	SEE REMARK 999	UNP G0S8G9
A	578	ASN	-	SEE REMARK 999	UNP G0S8G9
A	579	LYS	-	SEE REMARK 999	UNP G0S8G9
A	580	ASP	-	SEE REMARK 999	UNP G0S8G9
A	581	GLY	-	SEE REMARK 999	UNP G0S8G9
A	582	LYS	-	SEE REMARK 999	UNP G0S8G9
A	583	PHE	-	SEE REMARK 999	UNP G0S8G9
A	584	GLU	-	SEE REMARK 999	UNP G0S8G9
A	585	PHE	-	SEE REMARK 999	UNP G0S8G9
A	586	LYS	-	SEE REMARK 999	UNP G0S8G9
A	587	VAL	-	SEE REMARK 999	UNP G0S8G9
A	588	PRO	-	SEE REMARK 999	UNP G0S8G9
A	589	GLY	-	SEE REMARK 999	UNP G0S8G9
A	590	LEU	-	SEE REMARK 999	UNP G0S8G9
A	591	LEU	-	SEE REMARK 999	UNP G0S8G9
A	592	ILE	-	SEE REMARK 999	UNP G0S8G9
A	593	ILE	-	SEE REMARK 999	UNP G0S8G9
A	594	ASP	-	SEE REMARK 999	UNP G0S8G9
A	595	THR	-	SEE REMARK 999	UNP G0S8G9
A	596	PRO	-	SEE REMARK 999	UNP G0S8G9
A	597	GLY	-	SEE REMARK 999	UNP G0S8G9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	HIS	-	SEE REMARK 999	UNP G0S8G9
A	599	GLU	-	SEE REMARK 999	UNP G0S8G9
B	514	SER	-	EXPRESSION TAG	UNP G0S8G9
B	515	HIS	-	EXPRESSION TAG	UNP G0S8G9
B	516	MET	-	EXPRESSION TAG	UNP G0S8G9
B	576	VAL	-	SEE REMARK 999	UNP G0S8G9
B	577	VAL	-	SEE REMARK 999	UNP G0S8G9
B	578	ASN	-	SEE REMARK 999	UNP G0S8G9
B	579	LYS	-	SEE REMARK 999	UNP G0S8G9
B	580	ASP	-	SEE REMARK 999	UNP G0S8G9
B	581	GLY	-	SEE REMARK 999	UNP G0S8G9
B	582	LYS	-	SEE REMARK 999	UNP G0S8G9
B	583	PHE	-	SEE REMARK 999	UNP G0S8G9
B	584	GLU	-	SEE REMARK 999	UNP G0S8G9
B	585	PHE	-	SEE REMARK 999	UNP G0S8G9
B	586	LYS	-	SEE REMARK 999	UNP G0S8G9
B	587	VAL	-	SEE REMARK 999	UNP G0S8G9
B	588	PRO	-	SEE REMARK 999	UNP G0S8G9
B	589	GLY	-	SEE REMARK 999	UNP G0S8G9
B	590	LEU	-	SEE REMARK 999	UNP G0S8G9
B	591	LEU	-	SEE REMARK 999	UNP G0S8G9
B	592	ILE	-	SEE REMARK 999	UNP G0S8G9
B	593	ILE	-	SEE REMARK 999	UNP G0S8G9
B	594	ASP	-	SEE REMARK 999	UNP G0S8G9
B	595	THR	-	SEE REMARK 999	UNP G0S8G9
B	596	PRO	-	SEE REMARK 999	UNP G0S8G9
B	597	GLY	-	SEE REMARK 999	UNP G0S8G9
B	598	HIS	-	SEE REMARK 999	UNP G0S8G9
B	599	GLU	-	SEE REMARK 999	UNP G0S8G9

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	236	Total	O	0	5
			241	241		
7	B	272	Total	O	0	11
			283	283		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.41Å 114.84Å 65.88Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	46.65 – 1.87 46.65 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.65-1.87) 99.8 (46.65-1.87)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.164 , 0.204 0.167 , 0.207	Depositor DCC
R_{free} test set	3312 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 66297 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, GOL, MG, ACY, NA

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	0.86	0/2763	0.84	0/3726
1	B	0.85	2/2764 (0.1%)	0.80	2/3727 (0.1%)
All	All	0.85	2/5527 (0.0%)	0.82	2/7453 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	734	CYS	CB-SG	-5.75	1.72	1.81
1	B	646	ALA	CA-CB	5.26	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	MET	CG-SD-CE	5.71	109.34	100.20
1	B	729	LEU	CA-CB-CG	-5.14	103.47	115.30

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	2724	0	2789	26	0
1	B	2725	0	2784	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	0	12	0	0
2	B	32	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	18	0	24	3	0
5	B	24	0	32	8	0
6	B	4	0	3	2	0
7	A	241	0	0	5	0
7	B	283	0	0	4	0
All	All	6087	0	5656	61	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 5.

All (61) 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:B:559:GLN:NE2	1:B:754:GLU:OE2	2.21	0.73
1:A:707:ALA:HA	1:A:737:ARG:HD3	1.69	0.72
1:A:794:ARG:NH1	7:A:1308:HOH:O	2.20	0.72
1:B:637:ARG:NH1	1:B:693:GLN:O	2.29	0.65
1:B:732:GLN:NE2	7:B:1290:HOH:O	2.25	0.65
1:A:532:VAL:O	5:A:1005:GOL:H11	1.97	0.64
1:B:541:ASP:HB3	5:B:1006:GOL:H12	1.79	0.63
1:B:538:LYS:HE3	5:B:1006:GOL:H11	1.81	0.62
1:B:639[B]:ARG:NH1	7:B:1365:HOH:O	2.21	0.62
1:B:625:LEU:HD22	1:B:689:GLN:HB3	1.83	0.61
1:A:639[A]:ARG:NH2	7:A:1240:HOH:O	2.33	0.61
5:A:1004:GOL:H2	7:A:1126:HOH:O	2.02	0.60
1:A:790:LYS:HE3	1:A:852:GLU:OE2	2.03	0.59
1:A:625:LEU:HD22	1:A:689:GLN:HB3	1.86	0.58
1:B:588:PRO:HA	5:B:1005:GOL:H12	1.85	0.57
1:B:773:ILE:H	6:B:1004:ACY:H2	1.70	0.57
1:A:639[A]:ARG:NH1	7:A:1271:HOH:O	2.39	0.56
1:B:527:CYS:HB2	1:B:612:CYS:HB3	1.87	0.55
1:B:848:GLU:O	1:B:852:GLU:HG3	2.06	0.55
1:A:635:LEU:CD2	1:A:639[B]:ARG:HH12	2.20	0.54
1:B:763:VAL:HG11	1:B:831:GLU:HA	1.88	0.53
1:B:542:LYS:HA	5:B:1006:GOL:H32	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:VAL:HG13	1:B:733:LEU:HD11	1.91	0.53
1:A:779:ARG:CZ	1:A:790:LYS:HB3	2.42	0.50
1:B:541:ASP:CB	5:B:1006:GOL:H12	2.41	0.50
1:A:527:CYS:HB2	1:A:612:CYS:HB3	1.94	0.50
1:A:518:LYS:HA	1:A:521:LEU:HG	1.93	0.50
1:A:790:LYS:HE2	1:A:848:GLU:OE2	2.12	0.49
1:B:528[B]:ILE:HD12	1:B:616:ILE:HB	1.94	0.49
1:B:567:VAL:HG11	5:B:1005:GOL:H32	1.94	0.48
1:B:713:VAL:HG21	1:B:729:LEU:HD13	1.95	0.47
1:A:754:GLU:HG2	1:A:756:LYS:HG2	1.96	0.47
1:A:528[B]:ILE:CD1	1:A:616:ILE:HD12	2.45	0.46
1:A:647:LEU:HD21	1:A:686:VAL:HG11	1.97	0.46
1:A:756:LYS:HE2	1:A:824:LYS:HZ1	1.81	0.45
1:B:773:ILE:N	6:B:1004:ACY:H2	2.32	0.45
5:A:1006:GOL:H32	7:A:1203:HOH:O	2.15	0.45
1:A:779:ARG:HB3	1:A:842:VAL:CG2	2.46	0.45
1:B:713:VAL:CG2	1:B:729:LEU:HD13	2.46	0.45
1:B:538:LYS:CE	5:B:1006:GOL:H11	2.45	0.44
1:B:680:ARG:HH12	1:B:687:LYS:NZ	2.16	0.44
1:B:560:ILE:HG23	1:B:593:ILE:HG23	1.99	0.44
1:A:580:ASP:OD2	1:A:581:GLY:N	2.51	0.43
1:B:728:LYS:NZ	7:B:1322:HOH:O	2.52	0.43
1:B:785:LEU:HD23	1:B:785:LEU:HA	1.77	0.43
1:A:779:ARG:O	1:A:842:VAL:HG22	2.18	0.43
1:A:635:LEU:HD23	1:A:639[B]:ARG:HH12	1.82	0.43
1:B:696:ASN:HB3	1:B:709:TYR:CD2	2.54	0.43
1:A:713[A]:VAL:CG2	1:A:729:LEU:HD13	2.49	0.42
1:B:571:LYS:HG2	1:B:585:PHE:CD2	2.54	0.42
1:A:524:PRO:O	1:A:590:LEU:HD12	2.18	0.42
1:B:645:VAL:HG12	1:B:647:LEU:HD12	2.02	0.42
1:A:635:LEU:HD22	1:A:639[B]:ARG:HH12	1.84	0.42
1:A:779:ARG:HA	1:A:791:THR:O	2.21	0.41
1:B:680:ARG:HH12	1:B:687:LYS:HZ2	1.66	0.41
1:B:769:LEU:HG	1:B:819:ALA:HB2	2.02	0.41
1:B:680:ARG:O	1:B:680:ARG:HD2	2.21	0.41
1:B:783:CYS:SG	1:B:856:GLU:HA	2.61	0.41
1:A:779:ARG:NH2	1:A:790:LYS:HB3	2.36	0.40
1:A:756:LYS:HE2	1:A:824:LYS:NZ	2.36	0.40
5:B:1008:GOL:H12	7:B:1344[A]:HOH:O	2.21	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	346/457 (76%)	340 (98%)	6 (2%)	0	100	100
1	B	347/457 (76%)	341 (98%)	6 (2%)	0	100	100
All	All	693/914 (76%)	681 (98%)	12 (2%)	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	299/393 (76%)	294 (98%)	5 (2%)	68	61
1	B	299/393 (76%)	294 (98%)	5 (2%)	68	61
All	All	598/786 (76%)	588 (98%)	10 (2%)	68	61

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	550	GLU
1	A	658	LYS
1	A	779	ARG
1	A	790	LYS
1	A	821	GLN
1	B	658	LYS
1	B	680	ARG
1	B	782	LEU

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Mol	Chain	Res	Type
1	B	790	LYS
1	B	821	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	749	GLN

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	GTP	A	1001	3,4	25,34,34	1.02	2 (8%)	34,54,54	2.00	9 (26%)
5	GOL	A	1004	-	5,5,5	1.11	0	5,5,5	1.83	1 (20%)
5	GOL	A	1005	-	5,5,5	0.28	0	5,5,5	0.46	0
5	GOL	A	1006	-	5,5,5	0.58	0	5,5,5	0.33	0
2	GTP	B	1001	3,4	25,34,34	0.94	1 (4%)	34,54,54	2.00	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACY	B	1004	-	1,3,3	2.20	1 (100%)	0,3,3	0.00	-
5	GOL	B	1005	-	5,5,5	0.35	0	5,5,5	0.63	0
5	GOL	B	1006	-	5,5,5	0.22	0	5,5,5	0.90	0
5	GOL	B	1007	-	5,5,5	0.67	0	5,5,5	0.82	0
5	GOL	B	1008	-	5,5,5	1.01	0	5,5,5	1.58	1 (20%)

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	GTP	A	1001	3,4	-	0/18/38/38	0/3/3/3
5	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
2	GTP	B	1001	3,4	-	0/18/38/38	0/3/3/3
6	ACY	B	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1005	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1006	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1007	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1008	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GTP	C2-N1	2.09	1.39	1.35
6	B	1004	ACY	CH3-C	2.20	1.51	1.48
2	A	1001	GTP	C6-N1	2.81	1.38	1.33
2	B	1001	GTP	C8-N7	3.22	1.40	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GTP	N3-C2-N1	-5.90	118.46	127.44
2	B	1001	GTP	C2'-C1'-N9	-5.26	106.25	114.29
2	B	1001	GTP	C5-C6-N1	-4.25	117.78	123.59
2	B	1001	GTP	N3-C2-N1	-4.22	121.01	127.44
2	A	1001	GTP	C2'-C1'-N9	-4.12	108.00	114.29
2	B	1001	GTP	PA-O3A-PB	-3.90	121.79	132.73
2	A	1001	GTP	C6-C5-C4	-3.03	117.28	120.90
2	A	1001	GTP	C5-C6-N1	-2.63	120.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GTP	PA-O3A-PB	-2.45	125.84	132.73
2	A	1001	GTP	C1'-N9-C4	-2.30	123.47	126.94
2	B	1001	GTP	O3G-PG-O1G	2.12	117.41	110.58
2	B	1001	GTP	N2-C2-N1	2.16	120.78	117.20
5	B	1008	GOL	O1-C1-C2	2.16	120.67	110.18
2	B	1001	GTP	C4'-O4'-C1'	2.44	112.40	109.72
2	A	1001	GTP	O3G-PG-O2G	2.68	117.58	107.38
5	A	1004	GOL	C3-C2-C1	3.62	125.31	111.12
2	A	1001	GTP	C6-N1-C2	3.66	121.01	115.94
2	A	1001	GTP	N2-C2-N1	3.78	123.46	117.20
2	B	1001	GTP	C6-N1-C2	4.35	121.98	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1004	GOL	1	0
5	A	1005	GOL	1	0
5	A	1006	GOL	1	0
6	B	1004	ACY	2	0
5	B	1005	GOL	2	0
5	B	1006	GOL	5	0
5	B	1008	GOL	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.

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, 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	344/457 (75%)	-0.05	19 (5%) 29 30	14, 32, 79, 122	0
1	B	345/457 (75%)	-0.23	1 (0%) 94 94	15, 29, 63, 95	0
All	All	689/914 (75%)	-0.14	20 (2%) 55 57	14, 30, 72, 122	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	860	GLN	5.9
1	A	859	LEU	4.9
1	A	654	TYR	4.5
1	A	851	LEU	4.2
1	A	843	GLY	3.9
1	A	858	ASP	3.7
1	A	849	GLU	2.9
1	A	759	GLU	2.9
1	A	519	ASP	2.9
1	A	850	GLU	2.7
1	A	842	VAL	2.7
1	A	854	GLU	2.7
1	A	518	LYS	2.6
1	A	857	SER	2.4
1	A	844	PRO	2.4
1	A	846	ASP	2.4
1	A	847	ASP	2.2
1	A	853	GLU	2.1
1	B	858	ASP	2.1
1	A	688	LEU	2.0

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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	1005	6/6	0.81	0.35	21.75	37,51,54,56	0
5	GOL	B	1005	6/6	0.81	0.17	18.98	48,55,57,57	6
5	GOL	B	1006	6/6	0.84	0.18	7.30	37,52,57,65	0
5	GOL	B	1007	6/6	0.85	0.16	5.85	38,47,55,57	0
5	GOL	B	1008	6/6	0.85	0.14	4.79	26,45,48,52	0
6	ACY	B	1004	4/4	0.61	0.19	4.38	39,52,58,60	0
5	GOL	A	1004	6/6	0.88	0.18	4.11	27,28,40,55	0
5	GOL	A	1006	6/6	0.88	0.13	1.19	47,51,60,63	0
2	GTP	A	1001	32/32	0.99	0.08	-0.20	12,18,22,24	0
3	MG	B	1002	1/1	0.99	0.09	-0.61	18,18,18,18	0
2	GTP	B	1001	32/32	0.99	0.07	-0.70	15,19,24,27	0
4	NA	A	1003	1/1	0.98	0.06	-1.87	21,21,21,21	0
4	NA	B	1003	1/1	0.99	0.07	-1.98	20,20,20,20	0
3	MG	A	1002	1/1	0.99	0.06	-4.12	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.