Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:12 PM GMT

PDB ID	:	3WC0
Title	:	Crystal structure of C. albicans tRNA(His) guanylyltransferase (Thg1) with GTP
Authors	:	Nakamura, A.; Nemoto, T.; Sonoda, T.; Yamashita, K.; Tanaka, I.; Yao, M.
Deposited on	:	2013-05-24
Resolution	:	3.03 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:

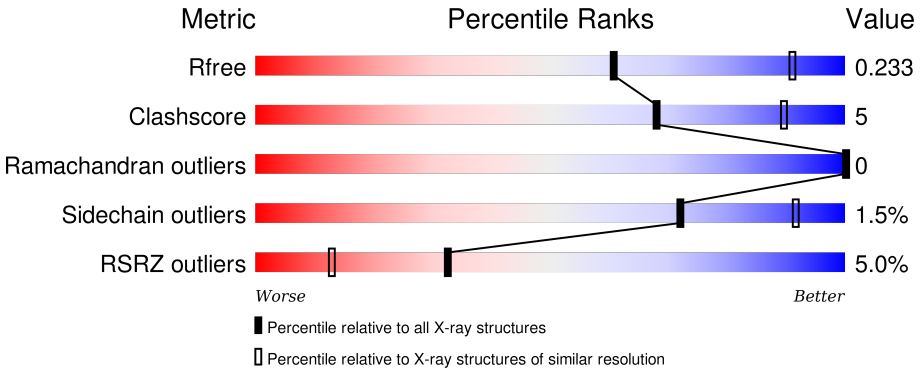
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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	271	6% 84% 14%
1	B	271	12% 86% 11%
1	C	271	3% 83% 14%
1	D	271	% 87% 11%
1	E	271	8% 73% 15% 11%

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Mol	Chain	Length	Quality of chain
1	F	271	75% 13% 11%
1	G	271	7% 86% 12%
1	H	271	5% 80% 18%
1	I	271	% 74% 15% 11%
1	J	271	7% 87% 10%
1	K	271	4% 83% 13%
1	L	271	% 77% 12% 11%
1	M	271	4% 82% 15%
1	N	271	4% 86% 11%
1	O	271	% 86% 11%
1	P	271	12% 78% 11% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36341 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 Likely histidyl tRNA-specific guanylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	B	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	C	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	D	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	E	241	Total	C	N	O	S	0	0	0
			2057	1337	335	373	12			
1	F	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			
1	G	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	H	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	I	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			
1	J	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	K	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	L	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			
1	M	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	N	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	O	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	P	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
A	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
A	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
B	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
B	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
B	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
C	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
C	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
C	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
D	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
D	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
D	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
E	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
E	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
E	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
F	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
F	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
F	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
G	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
G	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
G	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
H	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
H	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
H	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
I	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
I	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
I	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
J	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
J	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
J	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
K	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
K	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
K	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
L	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
L	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
L	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
M	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
M	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
M	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
N	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
N	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
N	0	SER	-	EXPRESSION TAG	UNP Q5AFK5

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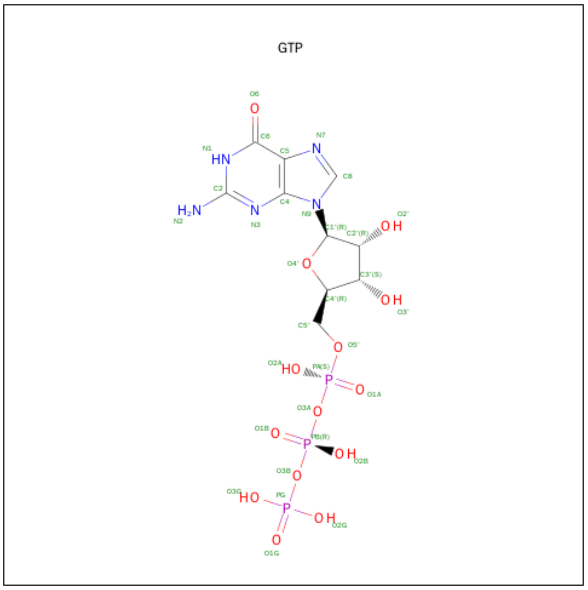
Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
O	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
O	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
P	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
P	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
P	0	SER	-	EXPRESSION TAG	UNP Q5AFK5

- 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	C	N	O	P	0	0
			32	10	5	14	3		
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	I	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	I	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	K	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	M	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	M	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	N	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	N	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	3	Total	Mg	0	0
			3	3		
3	G	3	Total	Mg	0	0
			3	3		
3	J	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	K	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	H	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	I	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	A	3	Total	Mg	0	0
			3	3		
3	N	3	Total	Mg	0	0
			3	3		
3	O	3	Total	Mg	0	0
			3	3		
3	L	4	Total	Mg	0	0
			4	4		
3	F	4	Total	Mg	0	0
			4	4		
3	M	3	Total	Mg	0	0
			3	3		

- Molecule 4 is water.

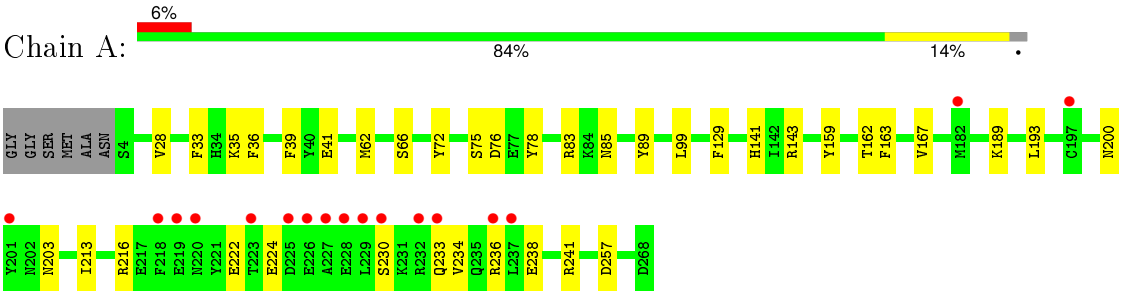
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total O 2 2	0	0
4	G	1	Total O 1 1	0	0
4	H	2	Total O 2 2	0	0
4	I	1	Total O 1 1	0	0
4	K	1	Total O 1 1	0	0
4	M	2	Total O 2 2	0	0
4	N	3	Total O 3 3	0	0
4	O	3	Total O 3 3	0	0

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 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.

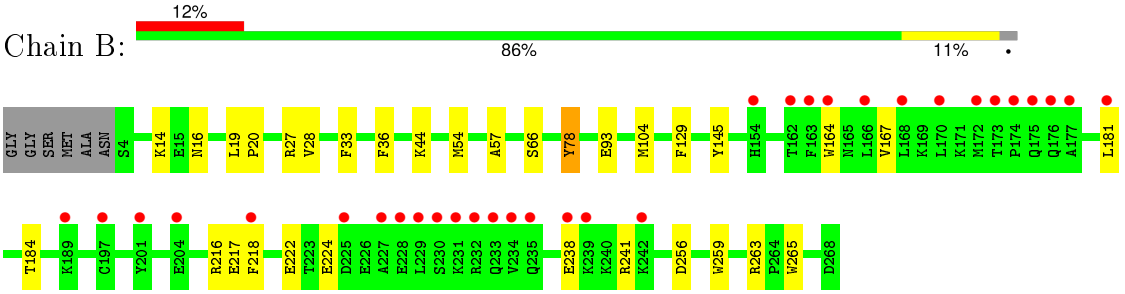
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain A:



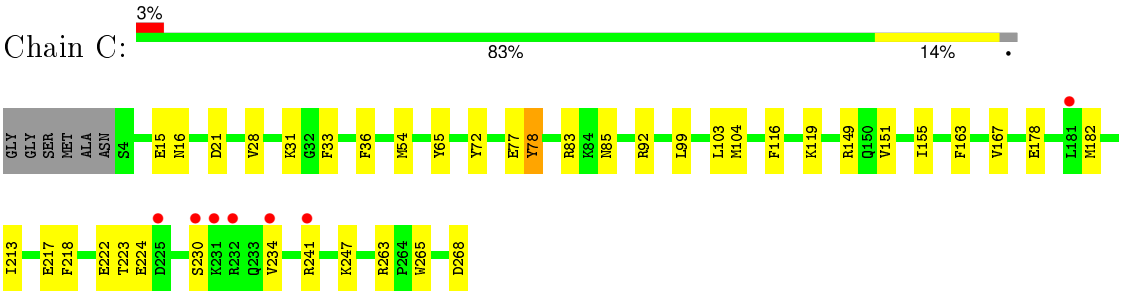
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain B:



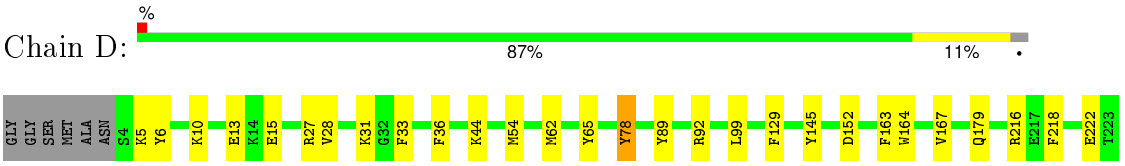
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

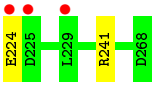
Chain C:



- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

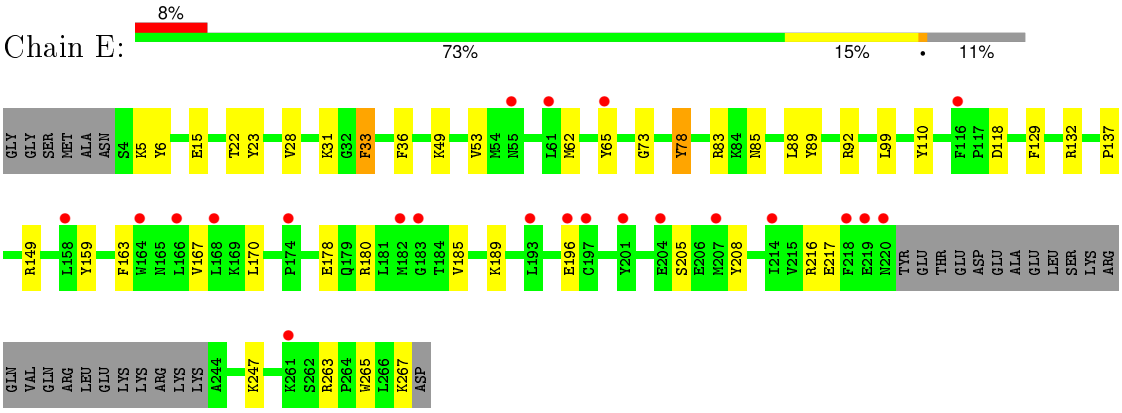
Chain D:





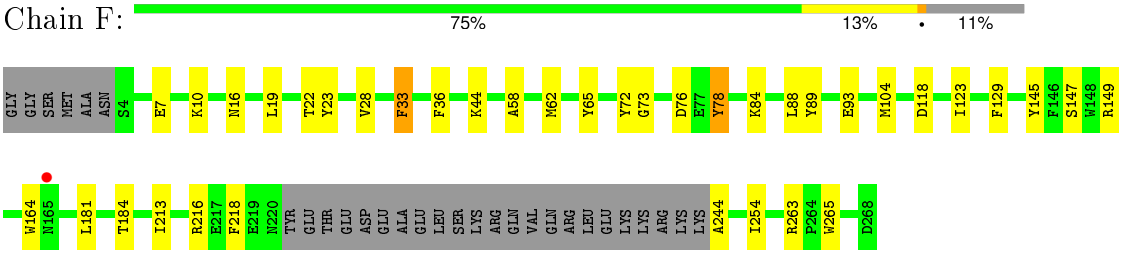
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain E:



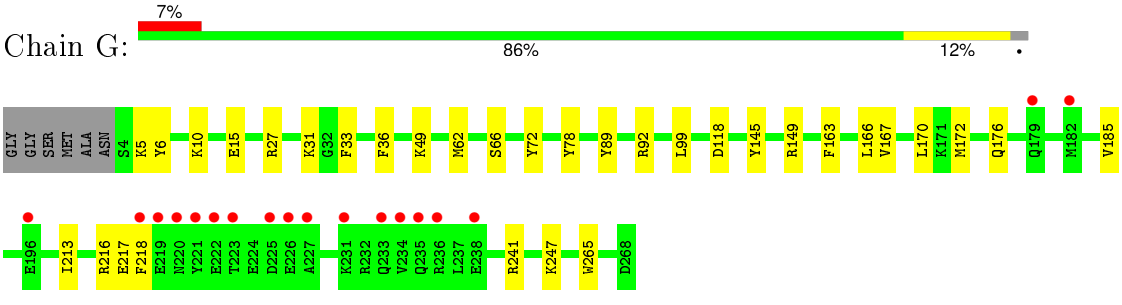
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain F:



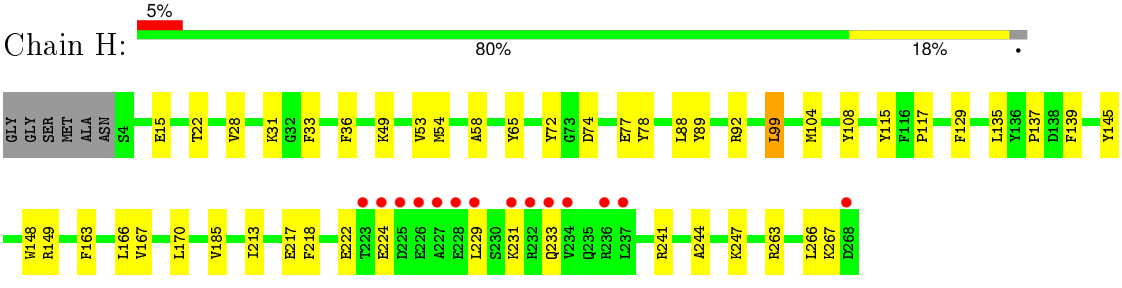
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain G:



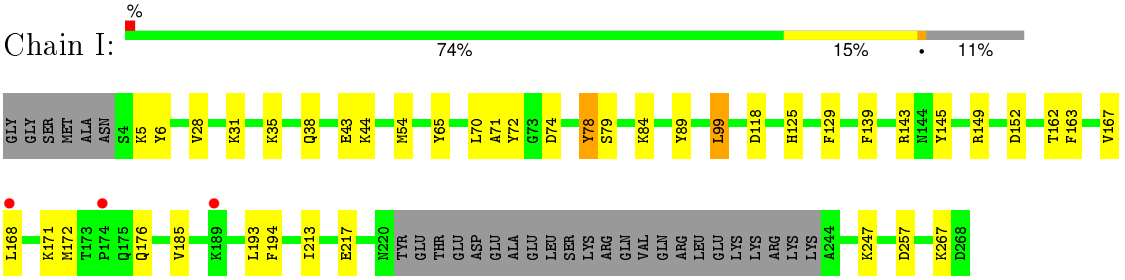
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain H:



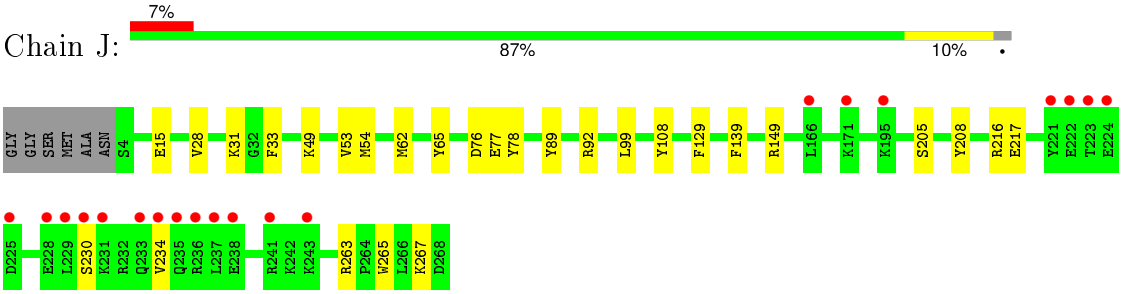
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain I:



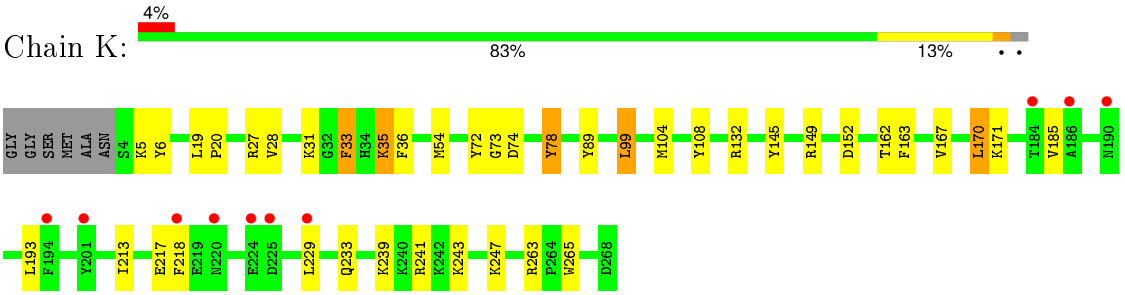
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain J:



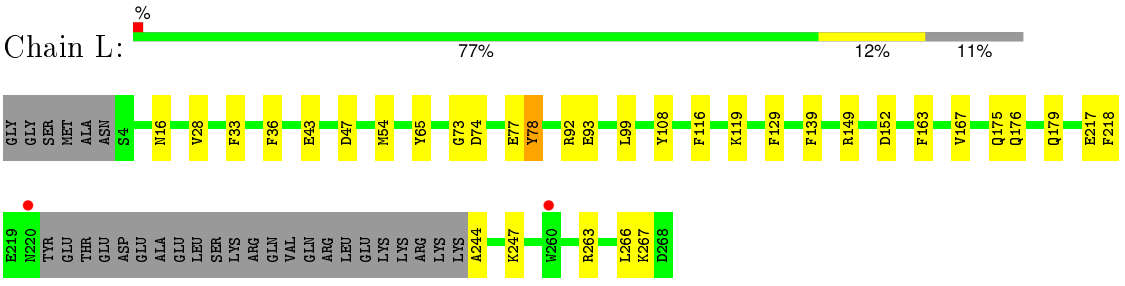
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain K:



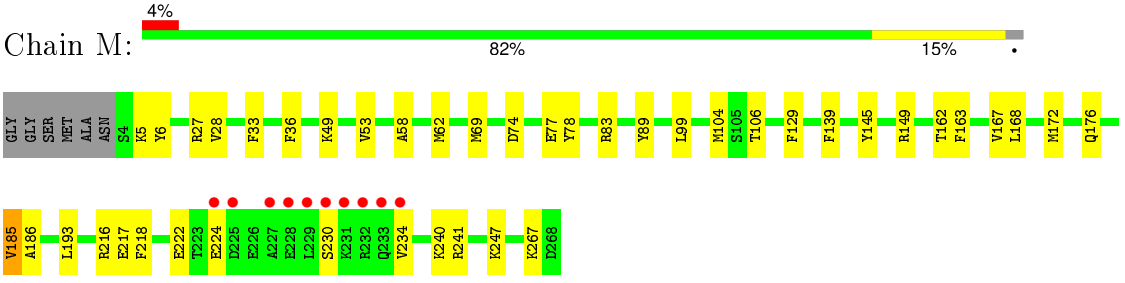
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain L:



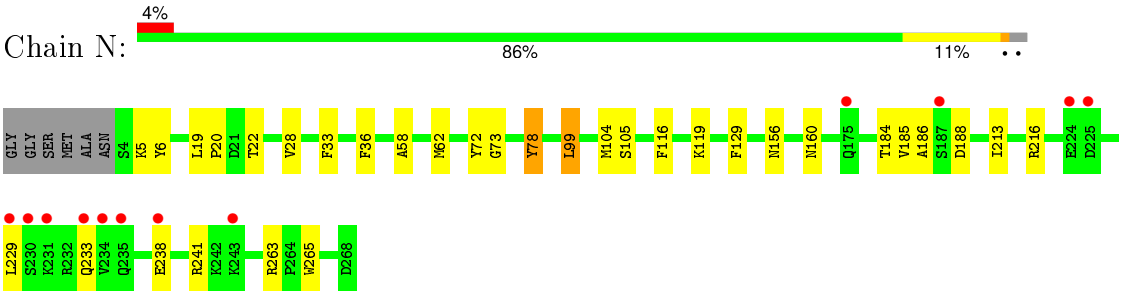
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain M:



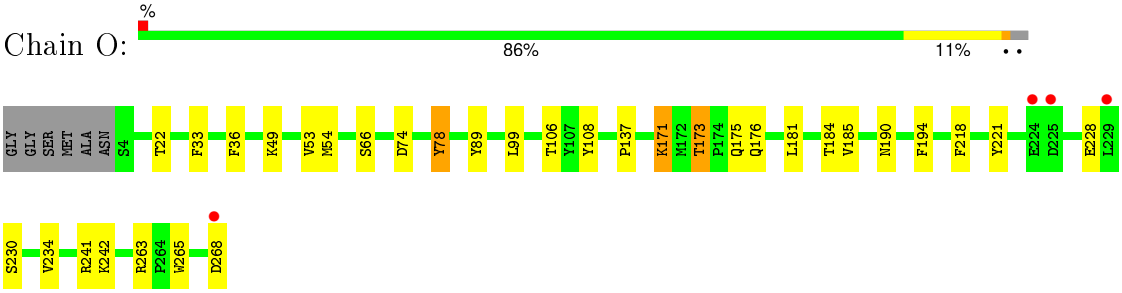
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain N:



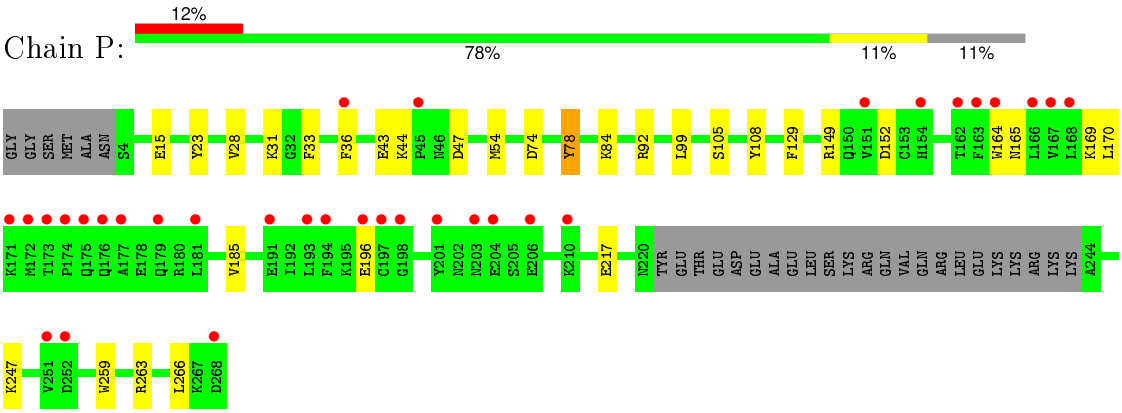
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain O:



• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.43Å 217.56Å 140.91Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	44.58 – 3.03 44.58 – 3.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.58-3.03) 98.9 (44.58-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.198 , 0.239 0.198 , 0.233	Depositor DCC
R_{free} test set	7035 reflections (7.14%)	DCC
Wilson B-factor (Å^2)	80.9	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 72.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 98553 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	36341	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: GTP, MG

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	0.28	0/2327	0.47	0/3135
1	B	0.29	0/2327	0.47	0/3135
1	C	0.29	0/2327	0.48	0/3135
1	D	0.30	0/2327	0.48	0/3135
1	E	0.29	0/2115	0.50	0/2854
1	F	0.31	0/2123	0.49	0/2865
1	G	0.30	0/2327	0.50	0/3135
1	H	0.31	0/2327	0.50	0/3135
1	I	0.31	0/2123	0.49	0/2865
1	J	0.29	0/2327	0.49	0/3135
1	K	0.31	0/2327	0.49	0/3135
1	L	0.30	0/2123	0.51	0/2865
1	M	0.32	0/2327	0.51	0/3135
1	N	0.33	0/2327	0.52	1/3135 (0.0%)
1	O	0.33	0/2327	0.52	0/3135
1	P	0.30	0/2123	0.48	0/2865
All	All	0.30	0/36204	0.49	1/48799 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	99	LEU	CA-CB-CG	-5.14	103.48	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	2267	0	2213	23	0
1	B	2267	0	2213	21	0
1	C	2267	0	2213	22	0
1	D	2267	0	2213	20	0
1	E	2057	0	1997	27	0
1	F	2065	0	2001	23	0
1	G	2267	0	2213	25	0
1	H	2267	0	2213	32	0
1	I	2065	0	2001	24	0
1	J	2267	0	2213	16	0
1	K	2267	0	2213	24	0
1	L	2065	0	2001	21	0
1	M	2267	0	2213	24	0
1	N	2267	0	2213	18	0
1	O	2267	0	2213	22	0
1	P	2065	0	2001	16	0
2	A	64	0	24	0	0
2	B	64	0	24	0	0
2	C	64	0	24	0	0
2	D	64	0	24	0	0
2	E	64	0	24	1	0
2	F	64	0	24	4	0
2	G	64	0	24	1	0
2	H	64	0	24	1	0
2	I	64	0	24	0	0
2	J	64	0	24	1	0
2	K	32	0	12	0	0
2	L	96	0	36	2	0
2	M	64	0	24	0	0
2	N	64	0	24	0	0
2	O	96	0	36	1	0
2	P	32	0	12	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	2	0	0	0	0
3	L	4	0	0	0	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	2	0	0	0	0
4	N	3	0	0	0	0
4	O	3	0	0	0	0
All	All	36341	0	34728	333	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 (333) 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:41:GLU:HG2	1:L:175:GLN:HE21	1.34	0.91
1:H:77:GLU:OE1	1:H:149:ARG:NH1	2.14	0.79
1:C:31:LYS:NZ	1:D:65:TYR:OH	2.21	0.74
1:P:263:ARG:HB3	1:P:266:LEU:HD13	1.70	0.73
1:L:92:ARG:NH1	2:L:301:GTP:O2G	2.25	0.70
1:K:31:LYS:NZ	1:L:65:TYR:OH	2.23	0.70
1:K:218:PHE:HZ	1:K:241:ARG:HG3	1.57	0.69
1:H:217:GLU:HG3	1:H:247:LYS:HD2	1.75	0.68
1:D:179:GLN:HG3	1:I:38:GLN:HE21	1.59	0.68
1:L:77:GLU:OE1	1:L:149:ARG:NH1	2.27	0.68
1:H:218:PHE:HZ	1:H:241:ARG:HG3	1.60	0.67
1:N:229:LEU:HD13	1:N:233:GLN:HE21	1.60	0.67
1:P:28:VAL:HG13	1:P:129:PHE:HB3	1.78	0.66
2:O:402:GTP:O1G	1:P:92:ARG:NH2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:VAL:HG13	1:J:129:PHE:HB3	1.77	0.65
1:F:10:LYS:HE2	2:F:301:GTP:C8	2.32	0.65
1:L:28:VAL:HG13	1:L:129:PHE:HB3	1.79	0.64
1:I:217:GLU:HG3	1:I:247:LYS:HD2	1.80	0.64
1:M:58:ALA:HA	1:M:104:MET:HE3	1.80	0.64
1:A:62:MET:O	1:A:216:ARG:NH2	2.31	0.63
1:A:159:TYR:HD1	1:A:189:LYS:HE2	1.63	0.63
1:J:217:GLU:OE2	1:J:263:ARG:NH1	2.31	0.63
1:K:28:VAL:HG21	1:K:104:MET:HG3	1.83	0.61
1:L:217:GLU:HG3	1:L:247:LYS:HD2	1.82	0.61
1:G:62:MET:O	1:G:216:ARG:NH2	2.33	0.60
1:C:217:GLU:HG3	1:C:247:LYS:HD2	1.83	0.60
1:J:89:TYR:HE2	1:J:99:LEU:HD22	1.67	0.60
1:K:218:PHE:CZ	1:K:241:ARG:HG3	2.37	0.60
1:O:54:MET:HG2	1:O:108:TYR:HE1	1.67	0.60
1:F:28:VAL:HG13	1:F:129:PHE:HB3	1.84	0.59
1:G:99:LEU:HD13	1:H:31:LYS:HE2	1.85	0.59
1:B:217:GLU:OE2	1:B:263:ARG:NH1	2.36	0.59
1:M:217:GLU:HG3	1:M:247:LYS:HD2	1.83	0.59
1:B:28:VAL:HG13	1:B:129:PHE:HB3	1.85	0.59
1:C:54:MET:HE3	1:C:78:TYR:HD2	1.68	0.58
1:P:33:PHE:HA	1:P:36:PHE:HB3	1.86	0.58
1:K:54:MET:HG2	1:K:108:TYR:HE1	1.69	0.58
1:H:229:LEU:HB3	1:H:233:GLN:HG3	1.86	0.58
1:C:218:PHE:HZ	1:C:241:ARG:HG3	1.68	0.57
1:I:143:ARG:NH2	1:I:257:ASP:OD1	2.38	0.57
1:B:218:PHE:HZ	1:B:241:ARG:HG3	1.69	0.57
1:A:41:GLU:HG2	1:L:175:GLN:NE2	2.11	0.57
1:E:217:GLU:HG3	1:E:247:LYS:HD2	1.87	0.57
1:N:156:ASN:O	1:N:160:ASN:ND2	2.36	0.57
1:E:28:VAL:HG13	1:E:129:PHE:HB3	1.87	0.56
1:D:163:PHE:O	1:D:167:VAL:HG23	2.04	0.56
1:A:89:TYR:HE2	1:A:99:LEU:HD22	1.70	0.56
1:A:33:PHE:HA	1:A:36:PHE:HB3	1.87	0.56
1:A:28:VAL:HG13	1:A:129:PHE:HB3	1.88	0.56
1:O:221:TYR:OH	1:O:268:ASP:OD2	2.23	0.56
1:F:16:ASN:ND2	1:F:93:GLU:OE1	2.34	0.56
1:A:75:SER:OG	1:A:76:ASP:N	2.38	0.56
1:M:218:PHE:HZ	1:M:241:ARG:HG3	1.71	0.56
1:I:35:LYS:HE2	1:I:125:HIS:NE2	2.21	0.55
1:J:54:MET:HG2	1:J:108:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:163:PHE:O	1:M:167:VAL:HG23	2.07	0.55
1:L:263:ARG:HB3	1:L:266:LEU:HD13	1.89	0.55
1:K:170:LEU:HD23	1:K:171:LYS:H	1.71	0.55
1:O:89:TYR:HE2	1:O:99:LEU:HD22	1.72	0.55
1:M:28:VAL:HG13	1:M:129:PHE:HB3	1.88	0.55
1:H:263:ARG:HB3	1:H:266:LEU:HD13	1.89	0.55
1:E:163:PHE:O	1:E:167:VAL:HG23	2.07	0.54
1:B:54:MET:HE3	1:B:78:TYR:HD2	1.72	0.54
1:P:54:MET:HG2	1:P:108:TYR:HE1	1.73	0.54
1:E:263:ARG:HG2	1:E:265:TRP:CZ2	2.41	0.54
1:P:44:LYS:HD3	1:P:164:TRP:CZ3	2.43	0.54
1:L:163:PHE:O	1:L:167:VAL:HG23	2.07	0.54
1:N:62:MET:O	1:N:216:ARG:NH2	2.41	0.54
1:O:230:SER:HA	1:O:234:VAL:HG23	1.90	0.54
1:G:33:PHE:HA	1:G:36:PHE:HB3	1.88	0.54
1:F:7:GLU:OE2	2:F:301:GTP:N2	2.41	0.54
1:K:229:LEU:HD22	1:K:233:GLN:HE21	1.73	0.54
1:D:179:GLN:HG3	1:I:38:GLN:NE2	2.21	0.53
1:C:77:GLU:OE1	1:C:149:ARG:NH2	2.42	0.53
1:D:222:GLU:O	1:D:224:GLU:N	2.38	0.53
1:O:173:THR:HG22	1:O:176:GLN:HG3	1.88	0.53
1:M:230:SER:HA	1:M:234:VAL:HG23	1.91	0.53
1:A:163:PHE:O	1:A:167:VAL:HG23	2.08	0.53
1:D:54:MET:HE3	1:D:78:TYR:HD2	1.73	0.53
1:A:143:ARG:NH2	1:A:257:ASP:OD1	2.41	0.53
1:K:89:TYR:HE2	1:K:99:LEU:HD22	1.73	0.53
1:A:39:PHE:O	1:L:176:GLN:HG2	2.09	0.53
1:E:89:TYR:HE2	1:E:99:LEU:HD22	1.73	0.52
1:N:28:VAL:HG13	1:N:129:PHE:HB3	1.90	0.52
1:B:14:LYS:NZ	1:C:16:ASN:OD1	2.23	0.52
1:M:89:TYR:HE2	1:M:99:LEU:HD22	1.74	0.52
1:L:16:ASN:ND2	1:L:93:GLU:OE1	2.42	0.52
1:O:263:ARG:HG2	1:O:265:TRP:CZ2	2.43	0.52
1:A:233:GLN:OE1	1:A:236:ARG:NH2	2.42	0.52
1:M:185:VAL:HG12	1:M:186:ALA:H	1.75	0.52
1:J:230:SER:HA	1:J:234:VAL:HG23	1.91	0.52
1:I:89:TYR:CE2	1:I:99:LEU:HD22	2.45	0.52
1:I:172:MET:HE2	1:I:176:GLN:HG2	1.92	0.52
1:G:99:LEU:HB2	1:H:31:LYS:NZ	2.25	0.52
1:B:27:ARG:HD3	1:B:145:TYR:OH	2.10	0.52
1:O:66:SER:HB3	1:O:242:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:VAL:HG13	1:I:129:PHE:HB3	1.92	0.51
1:L:116:PHE:CD1	1:L:119:LYS:HD2	2.45	0.51
1:I:72:TYR:HD1	1:I:213:ILE:HG13	1.75	0.51
1:N:185:VAL:HG22	1:N:186:ALA:H	1.75	0.51
1:H:54:MET:HG2	1:H:108:TYR:HE1	1.75	0.51
1:A:66:SER:HB2	1:A:241:ARG:HB3	1.92	0.51
1:E:5:LYS:HE3	1:E:6:TYR:CZ	2.44	0.51
1:H:163:PHE:O	1:H:167:VAL:HG23	2.10	0.51
1:M:218:PHE:CZ	1:M:241:ARG:HG3	2.46	0.51
1:P:54:MET:HE3	1:P:78:TYR:HD2	1.76	0.51
1:O:173:THR:HG23	1:O:175:GLN:H	1.75	0.51
1:J:77:GLU:OE2	1:J:149:ARG:NE	2.44	0.51
1:A:83:ARG:NH2	1:A:85:ASN:HB2	2.26	0.51
1:F:263:ARG:HG2	1:F:265:TRP:CZ2	2.46	0.51
1:H:28:VAL:HG13	1:H:129:PHE:HB3	1.93	0.50
1:E:65:TYR:CE2	1:E:99:LEU:HD21	2.45	0.50
1:F:62:MET:O	1:F:216:ARG:NH2	2.44	0.50
1:O:33:PHE:HA	1:O:36:PHE:HB3	1.92	0.50
1:A:230:SER:HA	1:A:234:VAL:HG23	1.94	0.50
1:J:263:ARG:HG2	1:J:265:TRP:CZ2	2.46	0.50
1:K:163:PHE:O	1:K:167:VAL:HG23	2.12	0.50
1:C:222:GLU:O	1:C:224:GLU:N	2.41	0.50
1:M:172:MET:HG2	1:M:176:GLN:HB2	1.93	0.50
1:E:31:LYS:NZ	1:F:65:TYR:OH	2.45	0.50
1:C:65:TYR:HE2	1:C:103:LEU:HD11	1.76	0.49
1:M:33:PHE:HA	1:M:36:PHE:HB3	1.93	0.49
1:M:162:THR:HA	1:M:193:LEU:HD21	1.94	0.49
1:A:141:HIS:NE2	1:C:21:ASP:OD2	2.27	0.49
1:M:62:MET:O	1:M:216:ARG:NH2	2.44	0.49
1:H:65:TYR:CE2	1:H:99:LEU:HD21	2.47	0.49
1:K:162:THR:HA	1:K:193:LEU:HD21	1.94	0.49
1:G:10:LYS:HD3	1:H:148:TRP:CH2	2.47	0.49
1:B:263:ARG:HG2	1:B:265:TRP:CZ2	2.48	0.49
1:I:89:TYR:HE2	1:I:99:LEU:HD22	1.77	0.49
1:E:92:ARG:NH2	2:E:404:GTP:O1G	2.36	0.49
1:C:263:ARG:HG2	1:C:265:TRP:CZ2	2.48	0.49
1:P:259:TRP:O	1:P:263:ARG:NH1	2.42	0.49
1:H:72:TYR:HD1	1:H:213:ILE:HG13	1.78	0.49
1:B:16:ASN:ND2	1:B:93:GLU:OE1	2.43	0.49
1:M:5:LYS:HE3	1:M:6:TYR:CZ	2.48	0.48
1:K:217:GLU:HG3	1:K:247:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:ARG:HH22	2:G:402:GTP:H4'	1.77	0.48
1:E:89:TYR:CE2	1:E:99:LEU:HD22	2.49	0.48
1:P:23:TYR:CE1	1:P:84:LYS:HB2	2.48	0.48
1:G:27:ARG:HD3	1:G:145:TYR:OH	2.13	0.48
1:O:171:LYS:HD2	1:O:171:LYS:N	2.29	0.48
1:K:132:ARG:NH2	2:L:301:GTP:O3G	2.43	0.48
1:G:99:LEU:HB2	1:H:31:LYS:HZ1	1.77	0.48
1:E:5:LYS:HE3	1:E:6:TYR:OH	2.14	0.48
1:N:5:LYS:HE3	1:N:6:TYR:CZ	2.49	0.48
1:J:89:TYR:CE2	1:J:99:LEU:HD22	2.48	0.48
1:N:263:ARG:HG2	1:N:265:TRP:CZ2	2.49	0.48
1:I:163:PHE:O	1:I:167:VAL:HG23	2.14	0.48
1:A:72:TYR:HD1	1:A:213:ILE:HG13	1.80	0.47
1:E:62:MET:O	1:E:216:ARG:NH2	2.47	0.47
1:F:88:LEU:HG	1:F:89:TYR:CD2	2.49	0.47
1:C:223:THR:HG23	1:C:268:ASP:OD2	2.15	0.47
1:D:44:LYS:HD3	1:D:164:TRP:CZ2	2.50	0.47
1:K:33:PHE:HA	1:K:36:PHE:HB3	1.95	0.47
1:B:164:TRP:HA	1:B:167:VAL:HG12	1.97	0.47
1:N:238:GLU:HG2	1:N:241:ARG:NH2	2.29	0.47
1:I:139:PHE:CD2	1:I:267:LYS:HG2	2.50	0.47
1:E:23:TYR:OH	1:E:267:LYS:O	2.24	0.47
1:M:27:ARG:HD3	1:M:145:TYR:OH	2.15	0.47
1:G:217:GLU:HG3	1:G:247:LYS:HD2	1.96	0.47
1:E:22:THR:HG23	1:E:137:PRO:HA	1.96	0.47
1:E:33:PHE:HA	1:E:36:PHE:HB3	1.97	0.47
1:G:89:TYR:HE2	1:G:99:LEU:HD22	1.80	0.47
1:O:218:PHE:CZ	1:O:241:ARG:HG3	2.50	0.47
1:H:89:TYR:CE2	1:H:99:LEU:HD22	2.49	0.46
1:P:217:GLU:HG3	1:P:247:LYS:HD2	1.95	0.46
1:E:132:ARG:NH2	2:F:301:GTP:O3G	2.46	0.46
1:K:5:LYS:HE3	1:K:6:TYR:CZ	2.51	0.46
1:J:15:GLU:CD	1:J:92:ARG:HH21	2.19	0.46
1:O:218:PHE:HD1	1:O:265:TRP:CG	2.34	0.46
1:G:163:PHE:O	1:G:167:VAL:HG23	2.16	0.46
1:N:19:LEU:HD23	1:N:22:THR:HG21	1.97	0.46
1:D:62:MET:O	1:D:216:ARG:NH2	2.47	0.46
1:N:184:THR:OG1	1:N:188:ASP:HB2	2.16	0.46
1:C:163:PHE:O	1:C:167:VAL:HG23	2.16	0.46
1:N:116:PHE:HB3	1:N:119:LYS:HB2	1.97	0.46
1:D:28:VAL:HG13	1:D:129:PHE:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:89:TYR:CE2	1:K:99:LEU:HD22	2.51	0.46
1:A:162:THR:HA	1:A:193:LEU:HD21	1.97	0.46
1:N:58:ALA:HA	1:N:104:MET:HE3	1.98	0.46
1:O:218:PHE:HZ	1:O:241:ARG:HG3	1.81	0.45
1:M:77:GLU:OE2	1:M:149:ARG:NE	2.49	0.45
1:F:44:LYS:HD3	1:F:164:TRP:CH2	2.50	0.45
1:H:88:LEU:HG	1:H:89:TYR:CD2	2.51	0.45
1:J:62:MET:O	1:J:216:ARG:NH2	2.49	0.45
1:C:99:LEU:HB2	1:D:31:LYS:NZ	2.32	0.45
1:D:218:PHE:HZ	1:D:241:ARG:HG3	1.82	0.45
1:C:151:VAL:O	1:C:155:ILE:HG12	2.16	0.45
1:C:178:GLU:O	1:C:182:MET:HG2	2.17	0.45
1:B:238:GLU:HG2	1:B:241:ARG:NH2	2.31	0.45
1:D:89:TYR:HE2	1:D:99:LEU:HD22	1.80	0.45
1:G:216:ARG:O	1:G:265:TRP:NE1	2.49	0.45
1:L:116:PHE:HB3	1:L:119:LYS:HB2	1.99	0.45
1:D:33:PHE:HA	1:D:36:PHE:HB3	1.98	0.45
1:J:49:LYS:O	1:J:53:VAL:HG23	2.17	0.45
1:D:5:LYS:HE3	1:D:6:TYR:CZ	2.52	0.45
1:K:73:GLY:HA3	1:K:78:TYR:CE2	2.51	0.45
1:J:205:SER:HB3	1:J:208:TYR:CD2	2.52	0.45
1:O:106:THR:HG23	1:P:105:SER:HB3	1.98	0.45
1:I:65:TYR:OH	1:J:31:LYS:NZ	2.49	0.45
1:J:139:PHE:CG	1:J:267:LYS:HG2	2.51	0.45
1:G:92:ARG:HH22	2:H:402:GTP:PG	2.39	0.44
1:L:33:PHE:HA	1:L:36:PHE:HB3	1.98	0.44
1:F:145:TYR:O	1:F:149:ARG:HG2	2.18	0.44
1:C:28:VAL:HG21	1:C:104:MET:HG3	1.99	0.44
1:P:165:ASN:O	1:P:169:LYS:HB2	2.17	0.44
1:B:181:LEU:O	1:B:184:THR:HG22	2.17	0.44
1:A:200:ASN:HD22	1:A:203:ASN:ND2	2.16	0.44
1:B:222:GLU:O	1:B:224:GLU:N	2.44	0.44
1:I:162:THR:HA	1:I:193:LEU:HD21	1.99	0.44
1:F:73:GLY:HA3	1:F:78:TYR:CE2	2.53	0.44
1:H:89:TYR:HE2	1:H:99:LEU:HD22	1.83	0.44
1:O:22:THR:HG23	1:O:137:PRO:HA	2.00	0.44
1:M:69:MET:CE	1:M:83:ARG:HD3	2.47	0.44
1:G:72:TYR:HD1	1:G:213:ILE:HG13	1.83	0.44
1:G:49:LYS:HE2	1:G:49:LYS:HB2	1.78	0.44
1:F:58:ALA:HA	1:F:104:MET:HE3	1.99	0.44
1:N:33:PHE:HA	1:N:36:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:LYS:O	1:M:53:VAL:HG23	2.17	0.44
1:M:222:GLU:O	1:M:224:GLU:N	2.43	0.44
1:K:54:MET:HE3	1:K:78:TYR:HD2	1.83	0.44
1:O:268:ASP:OD1	1:O:268:ASP:N	2.49	0.44
1:O:99:LEU:HB2	1:P:31:LYS:NZ	2.33	0.44
1:I:70:LEU:HD11	1:I:213:ILE:HG23	2.00	0.44
1:O:190:ASN:O	1:O:194:PHE:HD1	2.00	0.44
1:E:159:TYR:HD1	1:E:189:LYS:HE2	1.83	0.44
1:F:181:LEU:O	1:F:184:THR:HG22	2.18	0.43
1:G:172:MET:HE2	1:G:176:GLN:HB3	2.00	0.43
1:H:49:LYS:O	1:H:53:VAL:HG23	2.17	0.43
1:C:72:TYR:HD1	1:C:213:ILE:HG13	1.83	0.43
1:M:69:MET:HE3	1:M:83:ARG:HD3	2.00	0.43
1:F:33:PHE:HA	1:F:36:PHE:HB3	1.99	0.43
1:L:43:GLU:HB2	1:L:47:ASP:HA	2.00	0.43
1:E:205:SER:HB3	1:E:208:TYR:CD2	2.53	0.43
1:N:73:GLY:HA3	1:N:78:TYR:CE2	2.53	0.43
1:D:31:LYS:HE3	1:D:31:LYS:HB2	1.79	0.43
1:G:166:LEU:O	1:G:170:LEU:HB3	2.18	0.43
1:D:27:ARG:HD3	1:D:145:TYR:OH	2.18	0.43
1:H:222:GLU:O	1:H:224:GLU:N	2.44	0.43
1:E:15:GLU:OE1	1:E:92:ARG:HD2	2.18	0.43
1:N:20:PRO:O	1:N:22:THR:HG23	2.19	0.43
1:I:31:LYS:NZ	1:J:65:TYR:OH	2.52	0.43
1:J:76:ASP:OD1	2:J:401:GTP:O1A	2.37	0.43
1:I:43:GLU:HG3	1:I:44:LYS:N	2.33	0.43
1:H:139:PHE:CG	1:H:267:LYS:HG2	2.54	0.43
1:G:5:LYS:HE3	1:G:6:TYR:OH	2.18	0.43
1:C:33:PHE:HA	1:C:36:PHE:HB3	2.01	0.43
1:A:39:PHE:HD1	1:L:179:GLN:HB3	1.84	0.43
1:B:164:TRP:CE3	1:B:167:VAL:HG11	2.53	0.43
1:E:73:GLY:HA3	1:E:78:TYR:CE2	2.53	0.43
1:P:170:LEU:HD11	1:P:196:GLU:O	2.18	0.43
1:L:218:PHE:CE2	1:L:244:ALA:HB2	2.53	0.43
1:F:23:TYR:CD1	1:F:84:LYS:HB2	2.53	0.43
1:M:106:THR:CG2	1:N:105:SER:HB3	2.48	0.43
1:N:72:TYR:HD1	1:N:213:ILE:HG13	1.84	0.43
1:I:54:MET:HE3	1:I:78:TYR:HD2	1.84	0.43
1:G:89:TYR:CE2	1:G:99:LEU:HD22	2.54	0.42
1:G:31:LYS:HE2	1:H:65:TYR:OH	2.19	0.42
1:D:89:TYR:CE2	1:D:99:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:LEU:HD23	1:H:170:LEU:HA	1.87	0.42
1:H:218:PHE:CZ	1:H:241:ARG:HG3	2.47	0.42
1:G:5:LYS:HE3	1:G:6:TYR:CZ	2.54	0.42
1:H:58:ALA:HA	1:H:104:MET:HE3	2.02	0.42
1:D:44:LYS:HD3	1:D:164:TRP:CH2	2.55	0.42
1:E:83:ARG:NH2	1:E:85:ASN:HB2	2.34	0.42
1:B:216:ARG:O	1:B:265:TRP:NE1	2.52	0.42
1:H:15:GLU:OE1	1:H:92:ARG:HD2	2.20	0.42
1:F:72:TYR:HD1	1:F:213:ILE:HG13	1.85	0.42
1:D:10:LYS:HD2	1:D:13:GLU:OE2	2.20	0.42
1:L:73:GLY:HA3	1:L:78:TYR:CE2	2.54	0.42
1:C:230:SER:HA	1:C:234:VAL:HG23	2.01	0.42
1:F:218:PHE:CE2	1:F:244:ALA:HB2	2.55	0.42
1:L:139:PHE:CD2	1:L:267:LYS:HG2	2.55	0.42
1:K:35:LYS:HA	1:K:35:LYS:HE3	2.01	0.42
1:F:147:SER:HA	1:F:254:ILE:HG12	2.01	0.42
1:H:218:PHE:CE2	1:H:244:ALA:HB2	2.55	0.42
1:G:15:GLU:OE1	1:G:92:ARG:HD2	2.20	0.42
1:E:49:LYS:O	1:E:53:VAL:HG23	2.20	0.42
1:F:19:LEU:HD23	1:F:22:THR:HG21	2.01	0.41
1:M:89:TYR:CE2	1:M:99:LEU:HD22	2.54	0.41
1:C:83:ARG:NH1	1:C:85:ASN:HB2	2.35	0.41
1:K:72:TYR:HD1	1:K:213:ILE:HG13	1.85	0.41
1:H:33:PHE:HA	1:H:36:PHE:HB3	2.02	0.41
1:B:33:PHE:HA	1:B:36:PHE:HB3	2.01	0.41
1:O:181:LEU:O	1:O:184:THR:HG22	2.20	0.41
1:H:115:TYR:C	1:H:117:PRO:HD3	2.40	0.41
1:E:180:ARG:NH2	1:E:196:GLU:OE1	2.54	0.41
1:F:76:ASP:OD1	2:F:303:GTP:O1A	2.38	0.41
1:K:239:LYS:HE2	1:K:243:LYS:NZ	2.35	0.41
1:G:66:SER:HB2	1:G:241:ARG:HB3	2.03	0.41
1:O:173:THR:HG23	1:O:175:GLN:N	2.36	0.41
1:E:88:LEU:HG	1:E:89:TYR:CD2	2.55	0.41
1:I:217:GLU:HG3	1:I:247:LYS:CD	2.48	0.41
1:B:256:ASP:OD2	1:B:259:TRP:HB2	2.21	0.41
1:I:145:TYR:O	1:I:149:ARG:HG2	2.20	0.41
1:I:84:LYS:HB3	1:I:84:LYS:HE3	1.84	0.41
1:C:15:GLU:OE1	1:C:92:ARG:HD2	2.21	0.41
1:O:54:MET:HE3	1:O:78:TYR:HD2	1.85	0.41
1:A:35:LYS:HG3	1:L:179:GLN:HG3	2.02	0.41
1:M:139:PHE:CD2	1:M:267:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:TYR:O	1:K:149:ARG:HG2	2.21	0.41
1:N:99:LEU:HA	1:N:99:LEU:HD23	1.79	0.41
1:G:218:PHE:HZ	1:G:241:ARG:HG3	1.85	0.41
1:K:27:ARG:HD3	1:K:145:TYR:OH	2.20	0.41
1:E:110:TYR:CZ	1:F:123:ILE:HB	2.55	0.41
1:I:5:LYS:HE3	1:I:6:TYR:CZ	2.55	0.41
1:K:19:LEU:HA	1:K:20:PRO:HD3	1.93	0.41
1:P:43:GLU:HB2	1:P:47:ASP:HA	2.02	0.41
1:B:19:LEU:HA	1:B:20:PRO:HD3	1.89	0.41
1:H:145:TYR:O	1:H:148:TRP:HB3	2.21	0.40
1:B:66:SER:HB2	1:B:241:ARG:HB3	2.03	0.40
1:B:57:ALA:C	1:B:104:MET:HE1	2.41	0.40
1:I:118:ASP:N	1:I:118:ASP:OD1	2.51	0.40
1:A:222:GLU:O	1:A:224:GLU:N	2.47	0.40
1:I:71:ALA:HA	1:I:79:SER:O	2.21	0.40
1:P:15:GLU:OE1	1:P:92:ARG:HD2	2.22	0.40
1:A:234:VAL:O	1:A:238:GLU:HG3	2.21	0.40
1:F:22:THR:HG22	1:H:137:PRO:HB3	2.02	0.40
1:L:54:MET:HG2	1:L:108:TYR:HE1	1.87	0.40
1:F:118:ASP:N	1:F:118:ASP:OD1	2.53	0.40
1:G:118:ASP:N	1:G:118:ASP:OD1	2.53	0.40
1:C:116:PHE:HB3	1:C:119:LYS:HB2	2.02	0.40
1:H:22:THR:HG21	1:H:135:LEU:HB3	2.03	0.40
1:O:49:LYS:O	1:O:53:VAL:HG23	2.21	0.40
1:M:28:VAL:HG11	1:M:104:MET:HG3	2.04	0.40
1:B:218:PHE:CZ	1:B:241:ARG:HG3	2.51	0.40
1:B:44:LYS:HD3	1:B:164:TRP:CZ3	2.57	0.40
1:E:159:TYR:OH	1:E:178:GLU:OE2	2.38	0.40
1:H:166:LEU:HD23	1:H:170:LEU:HD12	2.03	0.40
1:D:15:GLU:OE1	1:D:92:ARG:HD2	2.22	0.40
1:E:118:ASP:OD1	1:E:118:ASP:N	2.55	0.40
1:K:263:ARG:HG2	1:K:265:TRP:CZ2	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	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	B	263/271 (97%)	254 (97%)	9 (3%)	0	100	100
1	C	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	D	263/271 (97%)	253 (96%)	10 (4%)	0	100	100
1	E	237/271 (88%)	233 (98%)	4 (2%)	0	100	100
1	F	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
1	G	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	H	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	I	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
1	J	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	K	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	L	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
1	M	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	N	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	O	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	P	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
All	All	4082/4336 (94%)	3971 (97%)	111 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/252 (99%)	248 (100%)	1 (0%)	93	98
1	B	249/252 (99%)	248 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	249/252 (99%)	248 (100%)	1 (0%)	93 98
1	D	249/252 (99%)	247 (99%)	2 (1%)	86 95
1	E	226/252 (90%)	221 (98%)	5 (2%)	60 87
1	F	227/252 (90%)	225 (99%)	2 (1%)	84 95
1	G	249/252 (99%)	247 (99%)	2 (1%)	86 95
1	H	249/252 (99%)	244 (98%)	5 (2%)	63 88
1	I	227/252 (90%)	219 (96%)	8 (4%)	43 79
1	J	249/252 (99%)	247 (99%)	2 (1%)	86 95
1	K	249/252 (99%)	241 (97%)	8 (3%)	46 81
1	L	227/252 (90%)	223 (98%)	4 (2%)	66 90
1	M	249/252 (99%)	244 (98%)	5 (2%)	63 88
1	N	249/252 (99%)	248 (100%)	1 (0%)	93 98
1	O	249/252 (99%)	243 (98%)	6 (2%)	57 86
1	P	227/252 (90%)	221 (97%)	6 (3%)	54 84
All	All	3873/4032 (96%)	3814 (98%)	59 (2%)	72 91

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	B	78	TYR
1	C	78	TYR
1	D	78	TYR
1	D	152	ASP
1	E	33	PHE
1	E	78	TYR
1	E	149	ARG
1	E	170	LEU
1	E	185	VAL
1	F	33	PHE
1	F	78	TYR
1	G	78	TYR
1	G	185	VAL
1	H	74	ASP
1	H	78	TYR
1	H	99	LEU
1	H	185	VAL

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Mol	Chain	Res	Type
1	H	231	LYS
1	I	74	ASP
1	I	78	TYR
1	I	99	LEU
1	I	152	ASP
1	I	168	LEU
1	I	171	LYS
1	I	185	VAL
1	I	194	PHE
1	J	33	PHE
1	J	78	TYR
1	K	33	PHE
1	K	35	LYS
1	K	74	ASP
1	K	78	TYR
1	K	99	LEU
1	K	152	ASP
1	K	170	LEU
1	K	185	VAL
1	L	74	ASP
1	L	78	TYR
1	L	99	LEU
1	L	152	ASP
1	M	74	ASP
1	M	78	TYR
1	M	168	LEU
1	M	185	VAL
1	M	240	LYS
1	N	78	TYR
1	O	74	ASP
1	O	78	TYR
1	O	171	LYS
1	O	173	THR
1	O	185	VAL
1	O	228	GLU
1	P	74	ASP
1	P	78	TYR
1	P	99	LEU
1	P	149	ARG
1	P	152	ASP
1	P	185	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	203	ASN
1	B	46	ASN
1	C	38	GLN
1	I	38	GLN
1	L	175	GLN
1	N	233	GLN
1	O	203	ASN
1	P	200	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 80 ligands modelled in this entry, 48 are monoatomic - leaving 32 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	401	3	25,34,34	0.94	1 (4%)	34,54,54	1.61	5 (14%)
2	GTP	A	402	3	25,34,34	0.89	1 (4%)	34,54,54	1.64	5 (14%)
2	GTP	B	401	3	25,34,34	0.93	1 (4%)	34,54,54	1.69	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GTP	B	402	3	25,34,34	0.90	1 (4%)	34,54,54	1.67	5 (14%)
2	GTP	C	401	3	25,34,34	0.94	1 (4%)	34,54,54	1.67	6 (17%)
2	GTP	C	405	3	25,34,34	0.91	1 (4%)	34,54,54	1.80	7 (20%)
2	GTP	D	301	3	25,34,34	0.92	1 (4%)	34,54,54	1.86	6 (17%)
2	GTP	D	302	3	25,34,34	0.94	1 (4%)	34,54,54	1.82	6 (17%)
2	GTP	E	401	3	25,34,34	0.89	1 (4%)	34,54,54	1.49	7 (20%)
2	GTP	E	404	3	25,34,34	0.95	2 (8%)	34,54,54	1.78	6 (17%)
2	GTP	F	301	3	25,34,34	0.91	1 (4%)	34,54,54	1.59	5 (14%)
2	GTP	F	303	3	25,34,34	0.96	1 (4%)	34,54,54	1.77	7 (20%)
2	GTP	G	401	3	25,34,34	0.94	1 (4%)	34,54,54	1.72	6 (17%)
2	GTP	G	402	3	25,34,34	0.88	1 (4%)	34,54,54	1.64	6 (17%)
2	GTP	H	401	3	25,34,34	0.95	1 (4%)	34,54,54	1.76	8 (23%)
2	GTP	H	402	3	25,34,34	0.90	2 (8%)	34,54,54	1.79	6 (17%)
2	GTP	I	401	3	25,34,34	0.95	1 (4%)	34,54,54	1.61	5 (14%)
2	GTP	I	402	3	25,34,34	0.90	1 (4%)	34,54,54	1.79	6 (17%)
2	GTP	J	401	3	25,34,34	0.93	1 (4%)	34,54,54	1.68	6 (17%)
2	GTP	J	402	3	25,34,34	0.92	1 (4%)	34,54,54	1.86	6 (17%)
2	GTP	K	401	3	25,34,34	0.93	1 (4%)	34,54,54	1.64	7 (20%)
2	GTP	L	301	3	25,34,34	0.92	2 (8%)	34,54,54	1.69	5 (14%)
2	GTP	L	303	3	25,34,34	0.97	1 (4%)	34,54,54	1.81	7 (20%)
2	GTP	L	304	3	25,34,34	0.89	1 (4%)	34,54,54	1.71	6 (17%)
2	GTP	M	401	3	25,34,34	0.99	2 (8%)	34,54,54	1.68	6 (17%)
2	GTP	M	402	3	25,34,34	0.89	1 (4%)	34,54,54	1.67	6 (17%)
2	GTP	N	401	3	25,34,34	0.96	2 (8%)	34,54,54	1.90	6 (17%)
2	GTP	N	402	3	25,34,34	0.91	1 (4%)	34,54,54	1.72	6 (17%)
2	GTP	O	401	3	25,34,34	0.95	1 (4%)	34,54,54	1.91	9 (26%)
2	GTP	O	402	3	25,34,34	0.87	1 (4%)	34,54,54	1.72	6 (17%)
2	GTP	O	406	3	25,34,34	0.92	1 (4%)	34,54,54	1.81	5 (14%)
2	GTP	P	401	3	25,34,34	0.94	1 (4%)	34,54,54	1.67	8 (23%)

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	401	3	-	0/18/38/38	0/3/3/3
2	GTP	A	402	3	-	0/18/38/38	0/3/3/3
2	GTP	B	401	3	-	0/18/38/38	0/3/3/3
2	GTP	B	402	3	-	0/18/38/38	0/3/3/3
2	GTP	C	401	3	-	0/18/38/38	0/3/3/3
2	GTP	C	405	3	-	0/18/38/38	0/3/3/3
2	GTP	D	301	3	-	0/18/38/38	0/3/3/3
2	GTP	D	302	3	-	0/18/38/38	0/3/3/3
2	GTP	E	401	3	-	0/18/38/38	0/3/3/3
2	GTP	E	404	3	-	0/18/38/38	0/3/3/3
2	GTP	F	301	3	-	0/18/38/38	0/3/3/3
2	GTP	F	303	3	-	0/18/38/38	0/3/3/3
2	GTP	G	401	3	-	0/18/38/38	0/3/3/3
2	GTP	G	402	3	-	0/18/38/38	0/3/3/3
2	GTP	H	401	3	-	0/18/38/38	0/3/3/3
2	GTP	H	402	3	-	0/18/38/38	0/3/3/3
2	GTP	I	401	3	-	0/18/38/38	0/3/3/3
2	GTP	I	402	3	-	0/18/38/38	0/3/3/3
2	GTP	J	401	3	-	0/18/38/38	0/3/3/3
2	GTP	J	402	3	-	0/18/38/38	0/3/3/3
2	GTP	K	401	3	-	0/18/38/38	0/3/3/3
2	GTP	L	301	3	-	0/18/38/38	0/3/3/3
2	GTP	L	303	3	-	0/18/38/38	0/3/3/3
2	GTP	L	304	3	-	0/18/38/38	0/3/3/3
2	GTP	M	401	3	-	0/18/38/38	0/3/3/3
2	GTP	M	402	3	-	0/18/38/38	0/3/3/3
2	GTP	N	401	3	-	0/18/38/38	0/3/3/3
2	GTP	N	402	3	-	0/18/38/38	0/3/3/3
2	GTP	O	401	3	-	0/18/38/38	0/3/3/3
2	GTP	O	402	3	-	0/18/38/38	0/3/3/3
2	GTP	O	406	3	-	0/18/38/38	0/3/3/3
2	GTP	P	401	3	-	0/18/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	GTP	C2-N1	2.00	1.38	1.35
2	N	401	GTP	C2-N1	2.04	1.39	1.35
2	H	402	GTP	C2-N1	2.05	1.39	1.35
2	E	404	GTP	C2-N1	2.09	1.39	1.35
2	M	401	GTP	C2-N1	2.09	1.39	1.35
2	G	402	GTP	C6-N1	2.59	1.37	1.33
2	O	402	GTP	C6-N1	2.60	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	402	GTP	C6-N1	2.68	1.38	1.33
2	L	301	GTP	C6-N1	2.68	1.38	1.33
2	F	301	GTP	C6-N1	2.69	1.38	1.33
2	L	304	GTP	C6-N1	2.69	1.38	1.33
2	B	402	GTP	C6-N1	2.71	1.38	1.33
2	M	402	GTP	C6-N1	2.73	1.38	1.33
2	A	402	GTP	C6-N1	2.73	1.38	1.33
2	C	405	GTP	C6-N1	2.73	1.38	1.33
2	I	402	GTP	C6-N1	2.75	1.38	1.33
2	J	402	GTP	C6-N1	2.76	1.38	1.33
2	N	402	GTP	C6-N1	2.80	1.38	1.33
2	O	406	GTP	C6-N1	2.82	1.38	1.33
2	E	404	GTP	C6-N1	2.83	1.38	1.33
2	G	401	GTP	C6-N1	2.86	1.38	1.33
2	J	401	GTP	C6-N1	2.86	1.38	1.33
2	D	302	GTP	C6-N1	2.86	1.38	1.33
2	E	401	GTP	C6-N1	2.87	1.38	1.33
2	D	301	GTP	C6-N1	2.89	1.38	1.33
2	B	401	GTP	C6-N1	2.89	1.38	1.33
2	C	401	GTP	C6-N1	2.92	1.38	1.33
2	K	401	GTP	C6-N1	2.93	1.38	1.33
2	H	401	GTP	C6-N1	2.97	1.38	1.33
2	A	401	GTP	C6-N1	2.98	1.38	1.33
2	O	401	GTP	C6-N1	2.99	1.38	1.33
2	P	401	GTP	C6-N1	2.99	1.38	1.33
2	I	401	GTP	C6-N1	3.04	1.38	1.33
2	M	401	GTP	C6-N1	3.04	1.38	1.33
2	F	303	GTP	C6-N1	3.04	1.38	1.33
2	N	401	GTP	C6-N1	3.11	1.38	1.33
2	L	303	GTP	C6-N1	3.17	1.39	1.33

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	401	GTP	C2'-C1'-N9	-6.34	104.60	114.29
2	O	401	GTP	C2'-C1'-N9	-5.72	105.55	114.29
2	D	302	GTP	C2'-C1'-N9	-5.33	106.15	114.29
2	L	303	GTP	C2'-C1'-N9	-5.18	106.38	114.29
2	M	402	GTP	N3-C2-N1	-5.17	119.57	127.44
2	I	402	GTP	N3-C2-N1	-5.16	119.58	127.44
2	D	301	GTP	N3-C2-N1	-5.15	119.60	127.44
2	O	401	GTP	N3-C2-N1	-5.10	119.68	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	406	GTP	PB-O3B-PG	-5.10	115.57	132.67
2	E	404	GTP	N3-C2-N1	-5.09	119.69	127.44
2	L	304	GTP	N3-C2-N1	-5.07	119.72	127.44
2	L	303	GTP	N3-C2-N1	-5.05	119.75	127.44
2	B	402	GTP	N3-C2-N1	-5.02	119.79	127.44
2	G	402	GTP	N3-C2-N1	-5.02	119.79	127.44
2	N	402	GTP	N3-C2-N1	-5.01	119.81	127.44
2	O	406	GTP	N3-C2-N1	-5.00	119.83	127.44
2	A	402	GTP	N3-C2-N1	-4.98	119.86	127.44
2	C	405	GTP	N3-C2-N1	-4.98	119.86	127.44
2	H	402	GTP	N3-C2-N1	-4.98	119.86	127.44
2	D	301	GTP	PA-O3A-PB	-4.94	118.85	132.73
2	J	402	GTP	N3-C2-N1	-4.93	119.93	127.44
2	F	301	GTP	N3-C2-N1	-4.93	119.94	127.44
2	O	402	GTP	N3-C2-N1	-4.89	120.00	127.44
2	F	303	GTP	N3-C2-N1	-4.89	120.00	127.44
2	I	401	GTP	N3-C2-N1	-4.84	120.07	127.44
2	L	301	GTP	N3-C2-N1	-4.84	120.07	127.44
2	K	401	GTP	N3-C2-N1	-4.83	120.08	127.44
2	I	402	GTP	PA-O3A-PB	-4.83	119.17	132.73
2	D	302	GTP	N3-C2-N1	-4.83	120.09	127.44
2	H	402	GTP	PA-O3A-PB	-4.82	119.20	132.73
2	C	401	GTP	N3-C2-N1	-4.80	120.13	127.44
2	A	401	GTP	N3-C2-N1	-4.79	120.15	127.44
2	J	402	GTP	PB-O3B-PG	-4.76	116.69	132.67
2	N	401	GTP	N3-C2-N1	-4.74	120.23	127.44
2	M	401	GTP	N3-C2-N1	-4.73	120.25	127.44
2	J	401	GTP	N3-C2-N1	-4.66	120.34	127.44
2	B	401	GTP	N3-C2-N1	-4.65	120.36	127.44
2	E	401	GTP	N3-C2-N1	-4.64	120.38	127.44
2	G	401	GTP	N3-C2-N1	-4.56	120.50	127.44
2	P	401	GTP	N3-C2-N1	-4.54	120.53	127.44
2	O	402	GTP	PA-O3A-PB	-4.47	120.19	132.73
2	G	401	GTP	C2'-C1'-N9	-4.45	107.49	114.29
2	H	401	GTP	N3-C2-N1	-4.45	120.67	127.44
2	L	304	GTP	PB-O3B-PG	-4.36	118.04	132.67
2	L	301	GTP	PB-O3B-PG	-4.31	118.22	132.67
2	D	301	GTP	PB-O3B-PG	-4.25	118.42	132.67
2	C	405	GTP	PA-O3A-PB	-4.15	121.09	132.73
2	F	301	GTP	PB-O3B-PG	-4.06	119.05	132.67
2	H	401	GTP	PA-O3A-PB	-4.01	121.48	132.73
2	J	402	GTP	PA-O3A-PB	-3.97	121.57	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	402	GTP	PA-O3A-PB	-3.95	121.64	132.73
2	N	402	GTP	PA-O3A-PB	-3.94	121.66	132.73
2	O	406	GTP	PA-O3A-PB	-3.88	121.83	132.73
2	B	402	GTP	PB-O3B-PG	-3.85	119.75	132.67
2	E	404	GTP	PB-O3B-PG	-3.84	119.78	132.67
2	E	404	GTP	PA-O3A-PB	-3.82	122.01	132.73
2	C	405	GTP	PB-O3B-PG	-3.81	119.90	132.67
2	C	401	GTP	C2'-C1'-N9	-3.77	108.53	114.29
2	J	401	GTP	PB-O3B-PG	-3.74	120.13	132.67
2	B	402	GTP	PA-O3A-PB	-3.71	122.32	132.73
2	L	301	GTP	PA-O3A-PB	-3.70	122.34	132.73
2	H	401	GTP	C2'-C1'-N9	-3.69	108.66	114.29
2	P	401	GTP	PB-O3B-PG	-3.68	120.34	132.67
2	O	402	GTP	PB-O3B-PG	-3.64	120.46	132.67
2	A	402	GTP	PB-O3B-PG	-3.63	120.50	132.67
2	A	401	GTP	C2'-C1'-N9	-3.62	108.76	114.29
2	G	402	GTP	PB-O3B-PG	-3.58	120.67	132.67
2	N	402	GTP	PB-O3B-PG	-3.57	120.70	132.67
2	F	303	GTP	PA-O3A-PB	-3.56	122.73	132.73
2	I	401	GTP	C2'-C1'-N9	-3.56	108.86	114.29
2	M	402	GTP	PB-O3B-PG	-3.53	120.83	132.67
2	H	402	GTP	PB-O3B-PG	-3.53	120.84	132.67
2	I	401	GTP	PB-O3B-PG	-3.53	120.85	132.67
2	J	402	GTP	C2'-C1'-N9	-3.48	108.97	114.29
2	B	401	GTP	PB-O3B-PG	-3.48	121.00	132.67
2	J	401	GTP	C2'-C1'-N9	-3.47	108.98	114.29
2	N	401	GTP	C5-C6-N1	-3.46	118.86	123.59
2	B	401	GTP	PA-O3A-PB	-3.44	123.08	132.73
2	B	401	GTP	C2'-C1'-N9	-3.41	109.08	114.29
2	F	303	GTP	C2'-C1'-N9	-3.40	109.10	114.29
2	I	402	GTP	PB-O3B-PG	-3.38	121.32	132.67
2	P	401	GTP	C5-C6-N1	-3.37	118.98	123.59
2	M	401	GTP	PA-O3A-PB	-3.37	123.27	132.73
2	P	401	GTP	PA-O3A-PB	-3.35	123.31	132.73
2	H	401	GTP	C5-C6-N1	-3.34	119.03	123.59
2	J	401	GTP	PA-O3A-PB	-3.31	123.43	132.73
2	D	302	GTP	PA-O3A-PB	-3.31	123.44	132.73
2	G	401	GTP	PA-O3A-PB	-3.27	123.56	132.73
2	F	303	GTP	PB-O3B-PG	-3.22	121.87	132.67
2	F	303	GTP	C5-C6-N1	-3.22	119.19	123.59
2	C	401	GTP	C5-C6-N1	-3.20	119.21	123.59
2	M	401	GTP	C2'-C1'-N9	-3.16	109.47	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	GTP	C2'-C1'-N9	-3.16	109.47	114.29
2	M	401	GTP	C5-C6-N1	-3.12	119.32	123.59
2	M	401	GTP	PB-O3B-PG	-3.05	122.43	132.67
2	B	401	GTP	C5-C6-N1	-3.05	119.42	123.59
2	L	304	GTP	PA-O3A-PB	-3.04	124.18	132.73
2	A	401	GTP	C5-C6-N1	-3.04	119.43	123.59
2	G	401	GTP	PB-O3B-PG	-3.03	122.51	132.67
2	A	402	GTP	PA-O3A-PB	-3.01	124.28	132.73
2	D	302	GTP	C5-C6-N1	-2.98	119.51	123.59
2	C	405	GTP	C5-C6-N1	-2.96	119.54	123.59
2	K	401	GTP	C5-C6-N1	-2.96	119.54	123.59
2	I	401	GTP	C5-C6-N1	-2.95	119.56	123.59
2	F	301	GTP	C5-C6-N1	-2.91	119.61	123.59
2	C	405	GTP	C2'-C1'-N9	-2.89	109.87	114.29
2	G	401	GTP	C5-C6-N1	-2.87	119.67	123.59
2	O	401	GTP	C5-C6-N1	-2.86	119.68	123.59
2	L	303	GTP	PA-O3A-PB	-2.85	124.72	132.73
2	K	401	GTP	PA-O3A-PB	-2.83	124.78	132.73
2	H	401	GTP	PB-O3B-PG	-2.83	123.19	132.67
2	E	401	GTP	C5-C6-N1	-2.82	119.73	123.59
2	L	303	GTP	C5-C6-N1	-2.81	119.75	123.59
2	J	401	GTP	C5-C6-N1	-2.80	119.75	123.59
2	O	401	GTP	PB-O3B-PG	-2.78	123.36	132.67
2	E	404	GTP	C5-C6-N1	-2.77	119.80	123.59
2	I	402	GTP	C5-C6-N1	-2.77	119.80	123.59
2	J	402	GTP	C5-C6-N1	-2.77	119.80	123.59
2	O	406	GTP	C5-C6-N1	-2.75	119.83	123.59
2	C	401	GTP	PB-O3B-PG	-2.75	123.45	132.67
2	D	302	GTP	PB-O3B-PG	-2.75	123.45	132.67
2	M	402	GTP	PA-O3A-PB	-2.74	125.04	132.73
2	A	402	GTP	C5-C6-N1	-2.73	119.85	123.59
2	H	402	GTP	C5-C6-N1	-2.72	119.86	123.59
2	L	301	GTP	C5-C6-N1	-2.69	119.90	123.59
2	L	304	GTP	C5-C6-N1	-2.69	119.92	123.59
2	D	301	GTP	C5-C6-N1	-2.68	119.92	123.59
2	K	401	GTP	PB-O3B-PG	-2.68	123.69	132.67
2	N	402	GTP	C5-C6-N1	-2.66	119.95	123.59
2	O	402	GTP	C5-C6-N1	-2.65	119.96	123.59
2	A	401	GTP	PA-O3A-PB	-2.62	125.38	132.73
2	L	304	GTP	C2'-C1'-N9	-2.59	110.33	114.29
2	B	402	GTP	C5-C6-N1	-2.58	120.06	123.59
2	G	402	GTP	C5-C6-N1	-2.51	120.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	GTP	PA-O3A-PB	-2.51	125.69	132.73
2	M	402	GTP	C5-C6-N1	-2.50	120.17	123.59
2	D	301	GTP	C2'-C1'-N9	-2.46	110.53	114.29
2	L	303	GTP	PB-O3B-PG	-2.42	124.57	132.67
2	I	402	GTP	C2'-C1'-N9	-2.40	110.62	114.29
2	C	401	GTP	PA-O3A-PB	-2.36	126.10	132.73
2	E	401	GTP	PB-O3B-PG	-2.32	124.87	132.67
2	O	401	GTP	PA-O3A-PB	-2.30	126.27	132.73
2	H	401	GTP	C4-C5-N7	-2.29	107.37	109.48
2	M	402	GTP	C1'-N9-C4	-2.28	123.50	126.94
2	P	401	GTP	C2'-C1'-N9	-2.28	110.81	114.29
2	N	401	GTP	C4-C5-N7	-2.18	107.47	109.48
2	E	401	GTP	PA-O3A-PB	-2.17	126.63	132.73
2	E	401	GTP	C2'-C1'-N9	-2.17	110.98	114.29
2	O	402	GTP	C2'-C1'-N9	-2.12	111.05	114.29
2	O	401	GTP	C1'-N9-C4	-2.03	123.88	126.94
2	N	402	GTP	C2'-C1'-N9	-2.03	111.20	114.29
2	C	405	GTP	C4'-O4'-C1'	2.02	111.94	109.72
2	K	401	GTP	O3A-PA-O5'	2.02	108.30	102.94
2	P	401	GTP	C4'-O4'-C1'	2.04	111.96	109.72
2	B	401	GTP	C4'-O4'-C1'	2.05	111.97	109.72
2	P	401	GTP	N2-C2-N1	2.06	120.60	117.20
2	F	303	GTP	N2-C2-N1	2.07	120.62	117.20
2	H	401	GTP	N2-C2-N1	2.09	120.67	117.20
2	O	401	GTP	O3A-PA-O5'	2.10	108.51	102.94
2	E	404	GTP	N2-C2-N1	2.13	120.72	117.20
2	G	402	GTP	C4'-O4'-C1'	2.16	112.10	109.72
2	N	401	GTP	N2-C2-N1	2.19	120.82	117.20
2	E	401	GTP	C4'-O4'-C1'	2.20	112.14	109.72
2	H	402	GTP	C4'-O4'-C1'	2.37	112.33	109.72
2	O	401	GTP	N2-C2-N1	2.40	121.18	117.20
2	L	303	GTP	N2-C2-N1	2.47	121.29	117.20
2	G	401	GTP	C6-N1-C2	2.52	119.44	115.94
2	E	401	GTP	C6-N1-C2	2.65	119.61	115.94
2	J	401	GTP	C6-N1-C2	2.65	119.62	115.94
2	L	301	GTP	C6-N1-C2	2.71	119.70	115.94
2	G	402	GTP	C6-N1-C2	2.74	119.75	115.94
2	O	402	GTP	C6-N1-C2	2.75	119.76	115.94
2	B	401	GTP	C6-N1-C2	2.77	119.78	115.94
2	I	401	GTP	C6-N1-C2	2.78	119.79	115.94
2	H	401	GTP	C6-N1-C2	2.79	119.81	115.94
2	B	402	GTP	C6-N1-C2	2.81	119.84	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	GTP	C6-N1-C2	2.83	119.87	115.94
2	N	402	GTP	C6-N1-C2	2.85	119.90	115.94
2	J	402	GTP	C6-N1-C2	2.86	119.90	115.94
2	A	402	GTP	C6-N1-C2	2.86	119.91	115.94
2	O	406	GTP	C6-N1-C2	2.87	119.92	115.94
2	D	302	GTP	C6-N1-C2	2.88	119.94	115.94
2	H	402	GTP	C6-N1-C2	2.89	119.94	115.94
2	P	401	GTP	C6-N1-C2	2.90	119.97	115.94
2	L	304	GTP	C6-N1-C2	2.91	119.98	115.94
2	L	303	GTP	C6-N1-C2	2.93	120.00	115.94
2	A	401	GTP	C6-N1-C2	2.94	120.02	115.94
2	M	401	GTP	C6-N1-C2	2.94	120.02	115.94
2	D	301	GTP	C6-N1-C2	2.96	120.05	115.94
2	M	402	GTP	C6-N1-C2	2.99	120.09	115.94
2	F	301	GTP	C6-N1-C2	3.00	120.10	115.94
2	E	404	GTP	C6-N1-C2	3.00	120.11	115.94
2	C	401	GTP	C6-N1-C2	3.03	120.14	115.94
2	O	401	GTP	C6-N1-C2	3.05	120.17	115.94
2	C	405	GTP	C6-N1-C2	3.05	120.17	115.94
2	I	402	GTP	C6-N1-C2	3.07	120.19	115.94
2	F	303	GTP	C6-N1-C2	3.12	120.27	115.94
2	N	401	GTP	C6-N1-C2	3.18	120.35	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	404	GTP	1	0
2	F	301	GTP	3	0
2	F	303	GTP	1	0
2	G	402	GTP	1	0
2	H	402	GTP	1	0
2	J	401	GTP	1	0
2	L	301	GTP	2	0
2	O	402	GTP	1	0

5.7 Other polymers

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

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	265/271 (97%)	0.30	17 (6%) 23 8	56, 90, 141, 156	0
1	B	265/271 (97%)	0.53	32 (12%) 6 2	50, 82, 139, 162	0
1	C	265/271 (97%)	0.12	7 (2%) 59 29	48, 92, 130, 138	0
1	D	265/271 (97%)	-0.12	3 (1%) 82 58	45, 69, 108, 128	0
1	E	241/271 (88%)	0.56	22 (9%) 11 4	44, 106, 147, 162	0
1	F	242/271 (89%)	0.04	1 (0%) 93 80	38, 67, 107, 126	0
1	G	265/271 (97%)	0.25	18 (6%) 20 7	38, 81, 139, 150	0
1	H	265/271 (97%)	0.07	14 (5%) 30 12	34, 65, 126, 146	0
1	I	242/271 (89%)	0.02	3 (1%) 81 55	40, 72, 119, 135	0
1	J	265/271 (97%)	0.35	20 (7%) 17 6	41, 82, 141, 162	0
1	K	265/271 (97%)	0.23	10 (3%) 44 19	36, 83, 142, 168	0
1	L	242/271 (89%)	-0.06	2 (0%) 87 68	48, 78, 110, 135	0
1	M	265/271 (97%)	0.06	10 (3%) 44 19	31, 59, 122, 139	0
1	N	265/271 (97%)	0.12	12 (4%) 37 15	28, 58, 120, 144	0
1	O	265/271 (97%)	-0.08	4 (1%) 76 49	40, 60, 118, 148	0
1	P	242/271 (89%)	0.79	33 (13%) 4 1	40, 93, 179, 188	0
All	All	4124/4336 (95%)	0.20	208 (5%) 32 13	28, 77, 137, 188	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	234	VAL	9.1
1	P	167	VAL	7.9
1	O	225	ASP	7.7
1	G	225	ASP	7.4
1	P	168	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
1	P	197	CYS	6.5
1	P	164	TRP	6.2
1	G	234	VAL	5.5
1	G	226	GLU	5.5
1	M	225	ASP	5.4
1	B	225	ASP	5.4
1	J	234	VAL	5.3
1	P	193	LEU	5.2
1	C	225	ASP	5.0
1	K	201	TYR	4.9
1	A	225	ASP	4.9
1	P	163	PHE	4.8
1	P	166	LEU	4.8
1	J	225	ASP	4.7
1	C	234	VAL	4.6
1	P	162	THR	4.6
1	H	225	ASP	4.6
1	J	230	SER	4.6
1	N	235	GLN	4.5
1	B	170	LEU	4.5
1	P	196	GLU	4.4
1	E	164	TRP	4.3
1	H	233	GLN	4.3
1	O	224	GLU	4.3
1	P	252	ASP	4.3
1	J	224	GLU	4.2
1	G	221	TYR	4.1
1	B	162	THR	4.1
1	P	268	ASP	4.0
1	P	198	GLY	4.0
1	P	191	GLU	4.0
1	B	234	VAL	3.9
1	B	235	GLN	3.9
1	A	233	GLN	3.9
1	J	235	GLN	3.9
1	E	174	PRO	3.9
1	C	231	LYS	3.9
1	C	230	SER	3.8
1	E	183	GLY	3.8
1	A	236	ARG	3.8
1	B	238	GLU	3.7
1	N	231	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	238	GLU	3.6
1	A	218	PHE	3.6
1	J	237	LEU	3.5
1	P	181	LEU	3.5
1	P	204	GLU	3.5
1	N	225	ASP	3.5
1	J	231	LYS	3.5
1	B	229	LEU	3.4
1	N	230	SER	3.4
1	B	227	ALA	3.4
1	A	201	TYR	3.4
1	K	225	ASP	3.4
1	P	174	PRO	3.4
1	M	231	LYS	3.4
1	E	218	PHE	3.4
1	B	174	PRO	3.4
1	J	221	TYR	3.4
1	P	171	LYS	3.3
1	M	228	GLU	3.3
1	G	220	ASN	3.3
1	A	226	GLU	3.3
1	B	177	ALA	3.3
1	P	172	MET	3.2
1	B	168	LEU	3.2
1	A	227	ALA	3.2
1	B	164	TRP	3.2
1	B	233	GLN	3.2
1	P	251	VAL	3.2
1	A	182	MET	3.1
1	H	231	LYS	3.1
1	B	201	TYR	3.1
1	P	45	PRO	3.1
1	B	189	LYS	3.1
1	M	233	GLN	3.1
1	K	186	ALA	3.0
1	H	229	LEU	3.0
1	P	201	TYR	3.0
1	B	166	LEU	3.0
1	N	175	GLN	2.9
1	J	233	GLN	2.9
1	G	236	ARG	2.9
1	B	232	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	268	ASP	2.9
1	G	219	GLU	2.9
1	D	225	ASP	2.9
1	M	230	SER	2.8
1	N	229	LEU	2.8
1	J	223	THR	2.8
1	H	232	ARG	2.8
1	B	230	SER	2.8
1	M	234	VAL	2.8
1	H	234	VAL	2.8
1	P	206	GLU	2.7
1	L	260	TRP	2.7
1	J	171	LYS	2.7
1	B	197	CYS	2.7
1	E	204	GLU	2.7
1	I	168	LEU	2.7
1	B	173	THR	2.7
1	J	166	LEU	2.7
1	J	243	LYS	2.7
1	A	230	SER	2.6
1	K	218	PHE	2.6
1	O	229	LEU	2.6
1	H	237	LEU	2.6
1	K	229	LEU	2.6
1	G	196	GLU	2.6
1	E	201	TYR	2.6
1	G	182	MET	2.6
1	E	220	ASN	2.6
1	K	194	PHE	2.6
1	B	154	HIS	2.5
1	A	232	ARG	2.5
1	J	222	GLU	2.5
1	A	229	LEU	2.5
1	B	181	LEU	2.5
1	H	227	ALA	2.5
1	D	224	GLU	2.5
1	P	203	ASN	2.5
1	K	190	ASN	2.5
1	K	220	ASN	2.5
1	B	228	GLU	2.5
1	P	210	LYS	2.5
1	A	228	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	55	ASN	2.5
1	N	243	LYS	2.5
1	G	223	THR	2.4
1	B	218	PHE	2.4
1	B	176	GLN	2.4
1	E	65	TYR	2.4
1	P	175	GLN	2.4
1	E	197	CYS	2.4
1	J	236	ARG	2.4
1	B	231	LYS	2.4
1	E	214	ILE	2.4
1	I	174	PRO	2.4
1	A	220	ASN	2.4
1	J	229	LEU	2.4
1	J	195	LYS	2.4
1	G	218	PHE	2.4
1	G	227	ALA	2.4
1	A	237	LEU	2.4
1	F	165	ASN	2.4
1	A	219	GLU	2.3
1	H	228	GLU	2.3
1	N	233	GLN	2.3
1	K	224	GLU	2.3
1	H	236	ARG	2.3
1	H	224	GLU	2.3
1	L	220	ASN	2.3
1	E	182	MET	2.3
1	B	163	PHE	2.3
1	E	61	LEU	2.3
1	M	227	ALA	2.3
1	E	219	GLU	2.3
1	G	222	GLU	2.3
1	P	176	GLN	2.3
1	E	193	LEU	2.3
1	P	179	GLN	2.3
1	P	173	THR	2.3
1	E	166	LEU	2.3
1	G	179	GLN	2.2
1	G	233	GLN	2.2
1	H	223	THR	2.2
1	B	242	LYS	2.2
1	B	172	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	194	PHE	2.2
1	P	151	VAL	2.2
1	J	241	ARG	2.2
1	M	232	ARG	2.2
1	E	261	LYS	2.2
1	J	228	GLU	2.2
1	E	116	PHE	2.2
1	E	168	LEU	2.2
1	A	197	CYS	2.2
1	A	223	THR	2.2
1	C	241	ARG	2.2
1	G	235	GLN	2.2
1	P	154	HIS	2.2
1	H	226	GLU	2.2
1	N	224	GLU	2.1
1	B	175	GLN	2.1
1	O	268	ASP	2.1
1	C	232	ARG	2.1
1	I	189	LYS	2.1
1	E	207	MET	2.1
1	N	238	GLU	2.1
1	G	238	GLU	2.1
1	B	204	GLU	2.0
1	E	196	GLU	2.0
1	M	224	GLU	2.0
1	E	158	LEU	2.0
1	M	229	LEU	2.0
1	P	177	ALA	2.0
1	B	239	LYS	2.0
1	G	231	LYS	2.0
1	C	181	LEU	2.0
1	D	229	LEU	2.0
1	P	36	PHE	2.0
1	N	187	SER	2.0
1	K	184	THR	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, 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	GTP	F	301	32/32	0.87	0.30	0.66	64,129,135,137	0
2	GTP	O	401	32/32	0.94	0.21	0.46	21,57,70,85	0
3	MG	O	404	1/1	0.88	0.20	0.21	27,27,27,27	0
2	GTP	H	402	32/32	0.94	0.23	0.15	26,92,99,101	0
2	GTP	C	405	32/32	0.92	0.22	0.12	40,103,115,121	0
2	GTP	O	402	32/32	0.94	0.24	0.12	22,113,118,118	0
2	GTP	C	401	32/32	0.94	0.23	-0.08	64,104,111,111	0
2	GTP	G	401	32/32	0.96	0.23	-0.15	45,84,90,92	0
2	GTP	E	404	32/32	0.95	0.21	-0.36	20,101,105,107	0
2	GTP	K	401	32/32	0.89	0.21	-0.39	129,146,177,177	0
2	GTP	L	303	32/32	0.94	0.19	-0.42	39,69,78,80	0
2	GTP	J	401	32/32	0.95	0.19	-0.44	43,69,74,75	0
2	GTP	N	401	32/32	0.97	0.17	-0.46	0,63,68,70	0
2	GTP	I	401	32/32	0.96	0.18	-0.47	10,93,102,127	0
2	GTP	F	303	32/32	0.95	0.21	-0.49	37,76,89,95	0
2	GTP	L	301	32/32	0.88	0.21	-0.59	123,138,167,192	0
2	GTP	D	302	32/32	0.96	0.17	-0.62	25,66,71,73	0
3	MG	N	404	1/1	0.99	0.16	-0.67	38,38,38,38	0
2	GTP	H	401	32/32	0.94	0.17	-0.67	30,57,66,66	0
2	GTP	D	301	32/32	0.94	0.20	-0.71	70,113,118,119	0
3	MG	E	403	1/1	0.89	0.19	-0.74	68,68,68,68	0
2	GTP	M	401	32/32	0.96	0.16	-0.77	25,55,68,72	0
3	MG	H	404	1/1	0.87	0.11	-0.80	29,29,29,29	0
2	GTP	L	304	32/32	0.96	0.19	-0.83	28,120,123,124	0
2	GTP	P	401	32/32	0.91	0.21	-0.84	58,101,113,116	0
3	MG	J	404	1/1	0.96	0.15	-0.85	47,47,47,47	0
2	GTP	G	402	32/32	0.95	0.21	-0.88	44,143,155,155	0
3	MG	A	404	1/1	0.98	0.15	-0.88	39,39,39,39	0
3	MG	F	305	1/1	0.93	0.19	-0.89	46,46,46,46	0
2	GTP	A	402	32/32	0.94	0.19	-0.90	43,122,128,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GTP	M	402	32/32	0.96	0.17	-0.91	31,95,104,106	0
2	GTP	B	401	32/32	0.92	0.18	-0.99	63,86,95,115	0
2	GTP	N	402	32/32	0.96	0.18	-1.01	18,114,121,123	0
2	GTP	J	402	32/32	0.97	0.19	-1.10	37,100,121,122	0
3	MG	C	403	1/1	0.99	0.07	-1.13	53,53,53,53	0
3	MG	D	304	1/1	0.83	0.14	-1.14	46,46,46,46	0
2	GTP	O	406	32/32	0.92	0.21	-1.14	39,129,133,134	0
3	MG	B	404	1/1	0.96	0.12	-1.15	42,42,42,42	0
2	GTP	E	401	32/32	0.91	0.19	-1.20	62,102,120,156	0
2	GTP	B	402	32/32	0.95	0.18	-1.27	59,123,126,126	0
2	GTP	I	402	32/32	0.95	0.18	-1.29	39,94,103,104	0
2	GTP	A	401	32/32	0.94	0.15	-1.53	60,81,91,96	0
3	MG	M	404	1/1	0.93	0.08	-1.65	16,16,16,16	0
3	MG	F	304	1/1	0.88	0.26	-	60,60,60,60	0
3	MG	A	405	1/1	0.95	0.21	-	45,45,45,45	0
3	MG	C	402	1/1	0.87	0.10	-	82,82,82,82	0
3	MG	E	402	1/1	0.98	0.24	-	91,91,91,91	0
3	MG	F	302	1/1	0.94	0.37	-	61,61,61,61	0
3	MG	G	403	1/1	0.80	0.17	-	69,69,69,69	0
3	MG	D	305	1/1	0.96	0.41	-	53,53,53,53	0
3	MG	B	403	1/1	0.88	0.16	-	71,71,71,71	0
3	MG	H	405	1/1	0.94	0.26	-	31,31,31,31	0
3	MG	L	302	1/1	0.93	0.15	-	74,74,74,74	0
3	MG	I	403	1/1	0.95	0.25	-	54,54,54,54	0
3	MG	C	404	1/1	0.91	0.17	-	54,54,54,54	0
3	MG	M	405	1/1	0.97	0.17	-	21,21,21,21	0
3	MG	J	405	1/1	0.92	0.29	-	43,43,43,43	0
3	MG	N	405	1/1	0.96	0.29	-	23,23,23,23	0
3	MG	G	405	1/1	0.95	0.32	-	50,50,50,50	0
3	MG	L	307	1/1	0.95	0.16	-	27,27,27,27	0
3	MG	J	403	1/1	0.90	0.19	-	54,54,54,54	0
3	MG	N	403	1/1	0.81	0.17	-	51,51,51,51	0
3	MG	P	403	1/1	0.93	0.21	-	42,42,42,42	0
3	MG	H	403	1/1	0.84	0.16	-	67,67,67,67	0
3	MG	P	404	1/1	0.97	0.26	-	42,42,42,42	0
3	MG	M	403	1/1	0.90	0.10	-	54,54,54,54	0
3	MG	O	403	1/1	0.77	0.22	-	48,48,48,48	0
3	MG	K	402	1/1	0.46	0.45	-	100,100,100,100	0
3	MG	P	402	1/1	0.89	0.10	-	65,65,65,65	0
3	MG	I	405	1/1	0.92	0.24	-	34,34,34,34	0
3	MG	B	405	1/1	0.98	0.23	-	56,56,56,56	0
3	MG	A	403	1/1	0.93	0.13	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	F	306	1/1	0.94	0.34	-	45,45,45,45	0
3	MG	I	404	1/1	0.99	0.16	-	61,61,61,61	0
3	MG	L	305	1/1	0.80	0.25	-	67,67,67,67	0
3	MG	D	303	1/1	0.83	0.10	-	77,77,77,77	0
3	MG	G	404	1/1	0.94	0.19	-	39,39,39,39	0
3	MG	K	403	1/1	0.88	0.13	-	220,220,220,220	0
3	MG	L	306	1/1	0.94	0.17	-	59,59,59,59	0
3	MG	O	405	1/1	0.87	0.23	-	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.