



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:22 PM GMT

PDB ID : 1A9C  
Title : GTP CYCLOHYDROLASE I (C110S MUTANT) IN COMPLEX WITH GTP  
Authors : Auerbach, G.; Nar, H.; Bracher, A.; Bacher, A.; Huber, R.  
Deposited on : 1998-04-04  
Resolution : 2.90 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

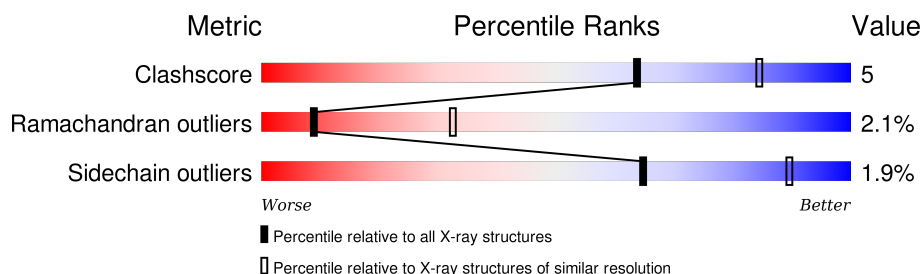
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)




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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	<div> <div>85%</div> <div>14%</div> </div>
1	B	221	<div> <div>83%</div> <div>17%</div> </div>
1	C	221	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	D	221	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	E	221	<div> <div>84%</div> <div>16%</div> </div>
1	F	221	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	G	221	<div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	221	 82% 17% •
1	I	221	 85% 14% •
1	J	221	 84% 16%
1	K	221	 86% 14%
1	L	221	 83% 16% •
1	M	221	 83% 17%
1	N	221	 83% 17%
1	O	221	 83% 16%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 33165 atoms, of which 6495 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.

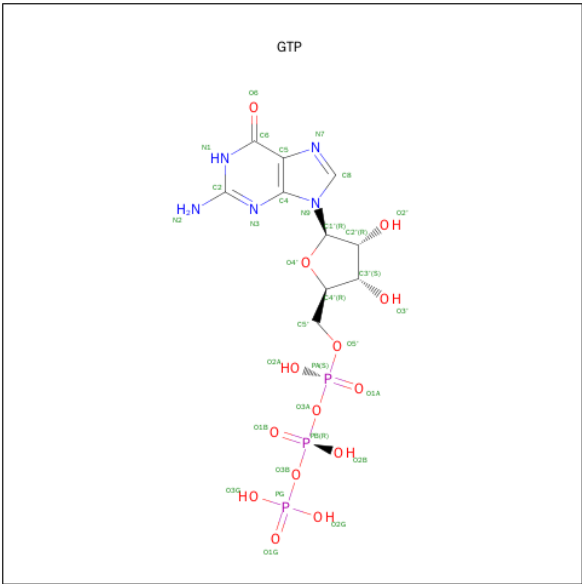
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	513	0	0
			2137	1088	405	309	327	8			
1	B	221	Total	C	H	N	O	S	510	0	0
			2137	1088	405	309	327	8			
1	C	221	Total	C	H	N	O	S	502	0	0
			2137	1088	405	309	327	8			
1	D	221	Total	C	H	N	O	S	502	0	0
			2137	1088	405	309	327	8			
1	E	221	Total	C	H	N	O	S	519	0	0
			2137	1088	405	309	327	8			
1	F	221	Total	C	H	N	O	S	527	0	0
			2137	1088	405	309	327	8			
1	G	221	Total	C	H	N	O	S	526	0	0
			2137	1088	405	309	327	8			
1	H	221	Total	C	H	N	O	S	513	0	0
			2137	1088	405	309	327	8			
1	I	221	Total	C	H	N	O	S	527	0	0
			2137	1088	405	309	327	8			
1	J	221	Total	C	H	N	O	S	502	0	0
			2137	1088	405	309	327	8			
1	K	221	Total	C	H	N	O	S	514	0	0
			2137	1088	405	309	327	8			
1	L	221	Total	C	H	N	O	S	531	0	0
			2137	1088	405	309	327	8			
1	M	221	Total	C	H	N	O	S	503	0	0
			2137	1088	405	309	327	8			
1	N	221	Total	C	H	N	O	S	519	0	0
			2137	1088	405	309	327	8			
1	O	221	Total	C	H	N	O	S	519	0	0
			2137	1088	405	309	327	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	CYS	MUTATION	UNP P0A6T5
B	110	SER	CYS	MUTATION	UNP P0A6T5
C	110	SER	CYS	MUTATION	UNP P0A6T5
D	110	SER	CYS	MUTATION	UNP P0A6T5
E	110	SER	CYS	MUTATION	UNP P0A6T5
F	110	SER	CYS	MUTATION	UNP P0A6T5
G	110	SER	CYS	MUTATION	UNP P0A6T5
H	110	SER	CYS	MUTATION	UNP P0A6T5
I	110	SER	CYS	MUTATION	UNP P0A6T5
J	110	SER	CYS	MUTATION	UNP P0A6T5
K	110	SER	CYS	MUTATION	UNP P0A6T5
L	110	SER	CYS	MUTATION	UNP P0A6T5
M	110	SER	CYS	MUTATION	UNP P0A6T5
N	110	SER	CYS	MUTATION	UNP P0A6T5
O	110	SER	CYS	MUTATION	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	14	Total	H	O	30	0
			42	28	14		
3	B	15	Total	H	O	32	0
			45	30	15		
3	C	14	Total	H	O	30	0
			42	28	14		
3	D	14	Total	H	O	30	0
			42	28	14		
3	E	13	Total	H	O	28	0
			39	26	13		
3	F	14	Total	H	O	30	0
			42	28	14		
3	G	13	Total	H	O	28	0
			39	26	13		
3	H	14	Total	H	O	30	0
			42	28	14		

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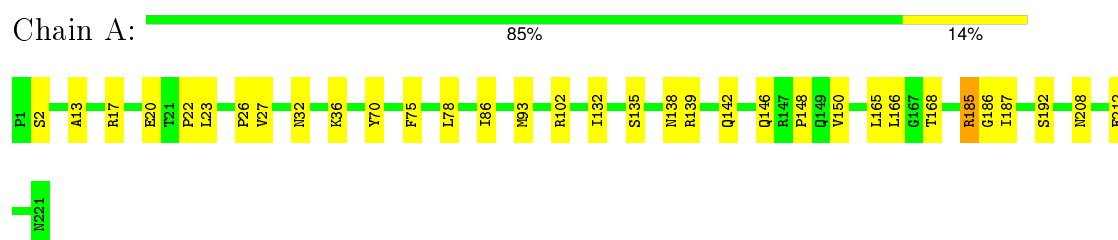
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	13	Total 39	H 26	O 13	28	0
3	J	16	Total 48	H 32	O 16	34	0
3	K	15	Total 45	H 30	O 15	32	0
3	L	13	Total 39	H 26	O 13	28	0
3	M	15	Total 45	H 30	O 15	33	0
3	N	14	Total 42	H 28	O 14	30	0
3	O	13	Total 39	H 26	O 13	28	0

### 3 Residue-property plots [i](#)

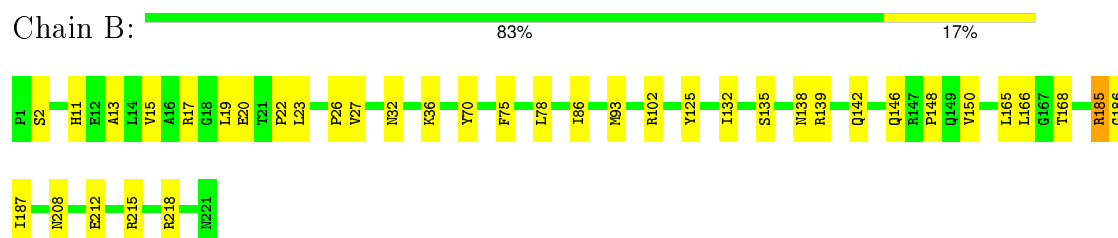
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

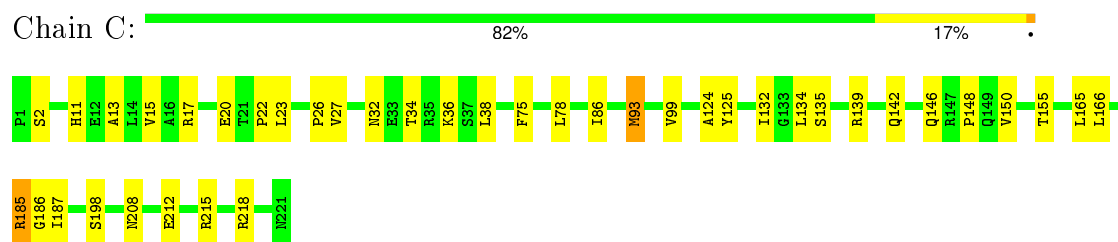
#### • Molecule 1: GTP CYCLOHYDROLASE I



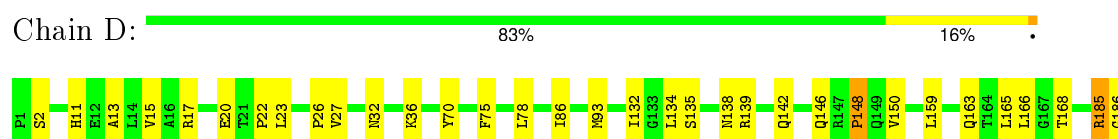
#### • Molecule 1: GTP CYCLOHYDROLASE I



#### • Molecule 1: GTP CYCLOHYDROLASE I



#### • Molecule 1: GTP CYCLOHYDROLASE I







• Molecule 1: GTP CYCLOHYDROLASE I

Chain E: 84% 16%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain F: 86% 13%



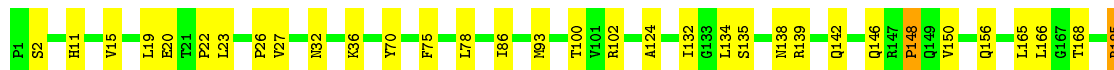
• Molecule 1: GTP CYCLOHYDROLASE I

Chain G: 85% 15%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain H: 82% 17%




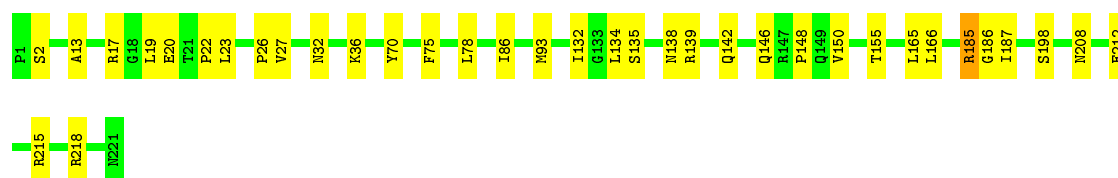
• Molecule 1: GTP CYCLOHYDROLASE I

Chain I: 85% 14%




• Molecule 1: GTP CYCLOHYDROLASE I

Chain J:  84% 16%




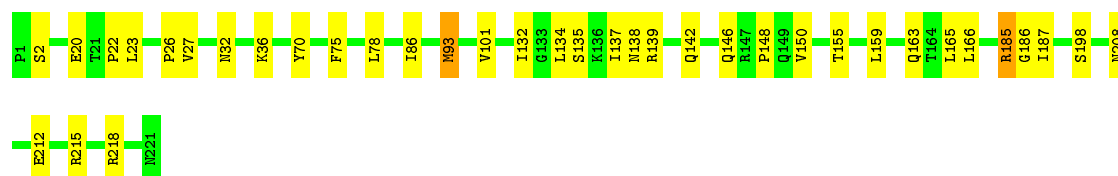
- Molecule 1: GTP CYCLOHYDROLASE I

Chain K:  86% 14%




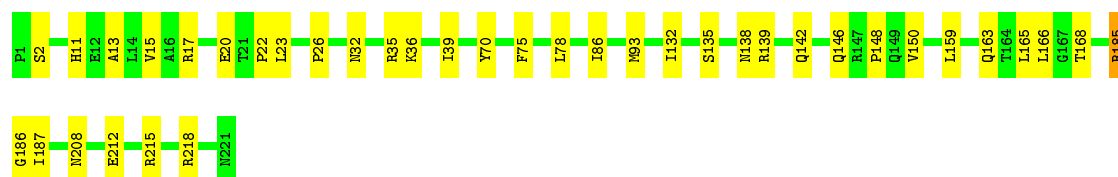
- Molecule 1: GTP CYCLOHYDROLASE I

Chain L:  83% 16%




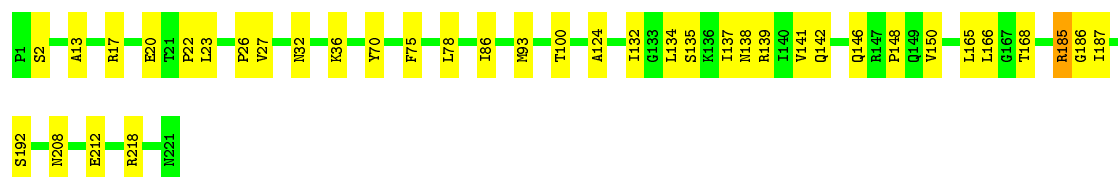
- Molecule 1: GTP CYCLOHYDROLASE I

Chain M:  83% 17%




- Molecule 1: GTP CYCLOHYDROLASE I

Chain N:  83% 17%



- Molecule 1: GTP CYCLOHYDROLASE I

Chain O:  83% 16%



S192	
S198	
E212	
R215	
R221	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	313.90Å 226.80Å 131.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	84.4 (8.00-2.90)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.206 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	0.47	0/1760	0.78	1/2384 (0.0%)
1	B	0.50	0/1760	0.78	1/2384 (0.0%)
1	C	0.51	0/1760	0.79	1/2384 (0.0%)
1	D	0.48	0/1760	0.78	2/2384 (0.1%)
1	E	0.46	0/1760	0.76	1/2384 (0.0%)
1	F	0.44	0/1760	0.74	1/2384 (0.0%)
1	G	0.44	0/1760	0.75	1/2384 (0.0%)
1	H	0.46	0/1760	0.77	2/2384 (0.1%)
1	I	0.43	0/1760	0.75	1/2384 (0.0%)
1	J	0.46	0/1760	0.76	1/2384 (0.0%)
1	K	0.44	0/1760	0.77	1/2384 (0.0%)
1	L	0.44	0/1760	0.75	1/2384 (0.0%)
1	M	0.45	0/1760	0.77	1/2384 (0.0%)
1	N	0.45	0/1760	0.76	1/2384 (0.0%)
1	O	0.45	0/1760	0.76	1/2384 (0.0%)
All	All	0.46	0/26400	0.76	17/35760 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	150	VAL	N-CA-C	-6.25	94.14	111.00
1	C	150	VAL	N-CA-C	-6.16	94.37	111.00
1	B	150	VAL	N-CA-C	-6.10	94.53	111.00
1	L	150	VAL	N-CA-C	-6.04	94.68	111.00
1	J	150	VAL	N-CA-C	-5.95	94.93	111.00
1	H	150	VAL	N-CA-C	-5.91	95.05	111.00
1	F	150	VAL	N-CA-C	-5.90	95.07	111.00
1	N	150	VAL	N-CA-C	-5.85	95.20	111.00
1	D	150	VAL	N-CA-C	-5.85	95.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	150	VAL	N-CA-C	-5.83	95.26	111.00
1	G	150	VAL	N-CA-C	-5.80	95.35	111.00
1	O	150	VAL	N-CA-C	-5.78	95.41	111.00
1	A	150	VAL	N-CA-C	-5.68	95.65	111.00
1	I	150	VAL	N-CA-C	-5.66	95.71	111.00
1	M	150	VAL	N-CA-C	-5.61	95.87	111.00
1	H	148	PRO	N-CA-C	-5.04	99.00	112.10
1	D	148	PRO	N-CA-C	-5.03	99.03	112.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1732	405	1768	18	0
1	B	1732	405	1768	21	0
1	C	1732	405	1768	23	0
1	D	1732	405	1768	18	0
1	E	1732	405	1768	20	0
1	F	1732	405	1768	16	0
1	G	1732	405	1768	17	0
1	H	1732	405	1768	23	0
1	I	1732	405	1768	20	0
1	J	1732	405	1768	19	0
1	K	1732	405	1768	20	0
1	L	1732	405	1768	21	0
1	M	1732	405	1768	21	0
1	N	1732	405	1768	20	0
1	O	1732	405	1768	21	0
2	A	32	0	12	0	0
2	B	32	0	12	1	0
2	C	32	0	12	1	0
2	D	32	0	12	0	0
2	E	32	0	12	0	0
2	F	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	32	0	12	1	0
2	H	32	0	12	0	0
2	I	32	0	12	1	0
2	J	32	0	12	1	0
2	K	32	0	12	1	0
2	L	32	0	12	0	0
2	M	32	0	12	1	0
2	N	32	0	12	1	0
2	O	32	0	12	1	0
3	A	14	28	0	0	0
3	B	15	30	0	0	0
3	C	14	28	0	0	0
3	D	14	28	0	0	0
3	E	13	26	0	0	0
3	F	14	28	0	0	0
3	G	13	26	0	0	0
3	H	14	28	0	0	0
3	I	13	26	0	0	0
3	J	16	32	0	0	0
3	K	15	30	0	0	0
3	L	13	26	0	0	0
3	M	15	30	0	0	0
3	N	14	28	0	0	0
3	O	13	26	0	0	0
All	All	26670	6495	26700	261	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 (261) 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:142:GLN:O	1:B:146:GLN:HG2	1.93	0.68
1:H:142:GLN:O	1:H:146:GLN:HG2	1.95	0.66
1:J:86:ILE:HG12	1:J:165:LEU:HD13	1.78	0.66
1:L:86:ILE:HG12	1:L:165:LEU:HD13	1.78	0.66
1:F:139:ARG:HG2	1:J:187:ILE:HD12	1.77	0.66
1:O:142:GLN:O	1:O:146:GLN:HG2	1.97	0.64
1:C:142:GLN:O	1:C:146:GLN:HG2	1.97	0.64
1:M:23:LEU:HD21	1:M:78:LEU:HD22	1.78	0.64
1:O:86:ILE:HG12	1:O:165:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:142:GLN:O	1:M:146:GLN:HG2	1.97	0.64
1:F:23:LEU:HD21	1:F:78:LEU:HD22	1.79	0.64
1:I:142:GLN:O	1:I:146:GLN:HG2	1.98	0.63
1:A:86:ILE:HG12	1:A:165:LEU:HD13	1.80	0.63
1:F:86:ILE:HG12	1:F:165:LEU:HD13	1.80	0.62
1:N:142:GLN:O	1:N:146:GLN:HG2	1.98	0.62
1:F:142:GLN:O	1:F:146:GLN:HG2	1.99	0.62
1:E:86:ILE:HG12	1:E:165:LEU:HD13	1.82	0.62
1:E:142:GLN:O	1:E:146:GLN:HG2	2.00	0.61
1:K:86:ILE:HG12	1:K:165:LEU:HD13	1.83	0.61
1:D:86:ILE:HG12	1:D:165:LEU:HD13	1.82	0.61
1:M:86:ILE:HG12	1:M:165:LEU:HD13	1.81	0.61
1:B:86:ILE:HG12	1:B:165:LEU:HD13	1.83	0.60
1:O:23:LEU:HD21	1:O:78:LEU:HD22	1.84	0.60
1:J:142:GLN:O	1:J:146:GLN:HG2	2.02	0.60
1:G:86:ILE:HG12	1:G:165:LEU:HD13	1.83	0.59
1:G:142:GLN:O	1:G:146:GLN:HG2	2.02	0.59
1:D:142:GLN:O	1:D:146:GLN:HG2	2.02	0.59
1:H:86:ILE:HG12	1:H:165:LEU:HD13	1.84	0.59
1:A:142:GLN:O	1:A:146:GLN:HG2	2.02	0.59
1:M:32:ASN:O	1:M:36:LYS:HG3	2.02	0.59
1:E:23:LEU:HD21	1:E:78:LEU:HD22	1.84	0.58
1:L:75:PHE:CE1	1:L:148:PRO:HG3	2.38	0.58
1:J:75:PHE:CE1	1:J:148:PRO:HG3	2.39	0.58
1:L:142:GLN:O	1:L:146:GLN:HG2	2.03	0.58
1:N:23:LEU:HD21	1:N:78:LEU:HD22	1.86	0.58
2:C:403:GTP:C2	1:D:134:LEU:HG	2.41	0.56
1:K:75:PHE:CE1	1:K:148:PRO:HG3	2.40	0.56
1:M:185:ARG:NH1	1:M:186:GLY:HA3	2.19	0.56
1:C:86:ILE:HG12	1:C:165:LEU:HD13	1.87	0.56
1:M:135:SER:O	1:M:139:ARG:HG3	2.06	0.56
1:N:86:ILE:HG12	1:N:165:LEU:HD13	1.86	0.56
1:K:23:LEU:HD21	1:K:78:LEU:HD22	1.88	0.56
1:A:138:ASN:HB3	1:E:187:ILE:HD13	1.88	0.55
1:E:75:PHE:CE1	1:E:148:PRO:HG3	2.40	0.55
1:I:86:ILE:HG12	1:I:165:LEU:HD13	1.88	0.55
1:F:135:SER:O	1:F:139:ARG:HG3	2.07	0.55
1:I:70:TYR:O	1:I:75:PHE:HB2	2.06	0.55
1:B:19:LEU:HD21	1:C:93:MET:HA	1.88	0.55
1:N:187:ILE:HD12	1:O:139:ARG:HG2	1.87	0.55
1:N:185:ARG:NH1	1:N:186:GLY:HA3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:187:ILE:HD12	1:L:139:ARG:HG2	1.88	0.55
1:F:132:ILE:HB	1:F:166:LEU:HD21	1.90	0.54
1:E:185:ARG:NH1	1:E:186:GLY:HA3	2.22	0.54
1:K:32:ASN:O	1:K:36:LYS:HG3	2.08	0.54
1:I:75:PHE:CE1	1:I:148:PRO:HG3	2.43	0.54
1:K:142:GLN:O	1:K:146:GLN:HG2	2.08	0.54
1:E:135:SER:O	1:E:139:ARG:HG3	2.08	0.54
1:N:75:PHE:CE1	1:N:148:PRO:HG3	2.43	0.54
1:H:23:LEU:HD21	1:H:78:LEU:HD22	1.90	0.53
1:M:185:ARG:HG2	1:M:186:GLY:N	2.24	0.53
1:C:185:ARG:HG2	1:C:186:GLY:N	2.23	0.53
1:K:185:ARG:NH1	1:K:186:GLY:HA3	2.23	0.53
1:D:23:LEU:HD21	1:D:78:LEU:HD22	1.89	0.53
1:H:75:PHE:CE1	1:H:148:PRO:HG3	2.44	0.53
1:I:187:ILE:HD12	1:J:139:ARG:HG2	1.90	0.53
1:B:23:LEU:HD21	1:B:78:LEU:HD22	1.91	0.53
1:E:132:ILE:HB	1:E:166:LEU:HD21	1.91	0.52
1:G:132:ILE:HB	1:G:166:LEU:HD21	1.91	0.52
1:A:187:ILE:HD12	1:B:139:ARG:HG2	1.89	0.52
1:D:132:ILE:HB	1:D:166:LEU:HD21	1.90	0.52
1:B:75:PHE:CE1	1:B:148:PRO:HG3	2.45	0.52
1:M:132:ILE:HB	1:M:166:LEU:HD21	1.91	0.52
1:I:132:ILE:HB	1:I:166:LEU:HD21	1.92	0.52
1:G:75:PHE:CE1	1:G:148:PRO:HG3	2.44	0.51
1:O:70:TYR:O	1:O:75:PHE:HB2	2.11	0.51
1:G:185:ARG:NH1	1:G:186:GLY:HA3	2.25	0.51
1:C:75:PHE:CE1	1:C:148:PRO:HG3	2.45	0.51
1:C:132:ILE:HB	1:C:166:LEU:HD21	1.93	0.51
1:M:187:ILE:HD13	1:N:138:ASN:HB3	1.93	0.51
1:D:185:ARG:NH1	1:D:186:GLY:HA3	2.25	0.51
1:K:139:ARG:HG2	1:O:187:ILE:HD12	1.92	0.51
1:O:132:ILE:HB	1:O:166:LEU:HD21	1.93	0.51
1:C:185:ARG:NH1	1:C:186:GLY:HA3	2.25	0.51
1:J:132:ILE:HB	1:J:166:LEU:HD21	1.92	0.51
1:F:93:MET:HA	1:J:19:LEU:HD21	1.92	0.51
1:F:185:ARG:NH1	1:F:186:GLY:HA3	2.26	0.51
1:F:187:ILE:HD12	1:G:139:ARG:HG2	1.93	0.51
1:A:23:LEU:HD21	1:A:78:LEU:HD22	1.92	0.51
1:L:185:ARG:NH1	1:L:186:GLY:HA3	2.26	0.50
1:F:75:PHE:CE1	1:F:148:PRO:HG3	2.47	0.50
1:I:185:ARG:NH1	1:I:186:GLY:HA3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:LEU:HD21	1:L:78:LEU:HD22	1.94	0.50
2:I:409:GTP:C2	1:J:134:LEU:HG	2.46	0.50
1:I:23:LEU:HD21	1:I:78:LEU:HD22	1.94	0.50
1:H:132:ILE:HB	1:H:166:LEU:HD21	1.93	0.50
1:G:185:ARG:HG2	1:G:186:GLY:N	2.27	0.49
1:D:185:ARG:HG2	1:D:186:GLY:N	2.27	0.49
1:K:132:ILE:HB	1:K:166:LEU:HD21	1.94	0.49
1:D:187:ILE:HD12	1:E:139:ARG:HG2	1.93	0.49
1:A:75:PHE:CE1	1:A:148:PRO:HG3	2.46	0.49
1:J:135:SER:O	1:J:139:ARG:HG3	2.12	0.49
1:F:100:THR:HG23	1:F:124:ALA:HB2	1.95	0.49
1:D:75:PHE:CE1	1:D:148:PRO:HG3	2.47	0.49
1:I:32:ASN:O	1:I:36:LYS:HG3	2.13	0.49
1:N:135:SER:O	1:N:139:ARG:HG3	2.12	0.49
1:L:135:SER:O	1:L:139:ARG:HG3	2.13	0.49
1:H:32:ASN:O	1:H:36:LYS:HG3	2.12	0.49
1:O:75:PHE:CE1	1:O:148:PRO:HG3	2.48	0.49
1:O:212:GLU:HG2	1:O:215:ARG:NH2	2.27	0.49
1:G:187:ILE:HD12	1:H:139:ARG:HG2	1.95	0.48
1:F:134:LEU:HG	2:J:410:GTP:C2	2.48	0.48
1:L:70:TYR:O	1:L:75:PHE:HB2	2.13	0.48
1:N:185:ARG:HG2	1:N:186:GLY:N	2.28	0.48
1:B:32:ASN:O	1:B:36:LYS:HG3	2.13	0.48
1:F:187:ILE:HD13	1:G:138:ASN:HB3	1.96	0.48
1:B:132:ILE:HB	1:B:166:LEU:HD21	1.95	0.48
1:F:185:ARG:HG2	1:F:186:GLY:N	2.28	0.48
1:J:70:TYR:O	1:J:75:PHE:HB2	2.13	0.48
1:N:132:ILE:HB	1:N:166:LEU:HD21	1.95	0.48
1:D:13:ALA:O	1:D:17:ARG:HD3	2.14	0.48
1:I:212:GLU:HG2	1:I:215:ARG:NH2	2.27	0.48
1:N:70:TYR:O	1:N:75:PHE:HB2	2.13	0.48
1:G:23:LEU:HD21	1:G:78:LEU:HD22	1.95	0.48
1:K:134:LEU:HG	2:O:415:GTP:C2	2.49	0.48
1:L:187:ILE:HD12	1:M:139:ARG:HG2	1.96	0.48
1:K:185:ARG:HG2	1:K:186:GLY:N	2.29	0.48
1:O:185:ARG:HG2	1:O:186:GLY:N	2.27	0.48
1:A:70:TYR:O	1:A:75:PHE:HB2	2.14	0.47
1:B:212:GLU:HG2	1:B:215:ARG:NH2	2.30	0.47
1:G:70:TYR:O	1:G:75:PHE:HB2	2.14	0.47
1:B:185:ARG:NH1	1:B:186:GLY:HA3	2.28	0.47
1:E:13:ALA:O	1:E:17:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ASN:O	1:E:36:LYS:HG3	2.14	0.47
1:E:185:ARG:HG2	1:E:186:GLY:N	2.30	0.47
1:E:212:GLU:HG2	1:E:215:ARG:NH2	2.30	0.47
1:L:132:ILE:HB	1:L:166:LEU:HD21	1.96	0.47
1:H:187:ILE:HD12	1:I:139:ARG:HG2	1.96	0.47
1:H:187:ILE:HD13	1:I:138:ASN:HB3	1.97	0.47
1:N:100:THR:HG23	1:N:124:ALA:HB2	1.97	0.47
1:C:23:LEU:HD21	1:C:78:LEU:HD22	1.96	0.47
1:M:13:ALA:O	1:M:17:ARG:HD3	2.15	0.47
1:D:70:TYR:O	1:D:75:PHE:HB2	2.15	0.46
2:N:414:GTP:C2	1:O:134:LEU:HG	2.50	0.46
1:B:70:TYR:O	1:B:75:PHE:HB2	2.15	0.46
1:L:159:LEU:O	1:L:163:GLN:HG3	2.15	0.46
1:G:212:GLU:HG2	1:G:215:ARG:NH2	2.30	0.46
1:I:135:SER:O	1:I:139:ARG:HG3	2.15	0.46
1:H:185:ARG:NH1	1:H:186:GLY:HA3	2.30	0.46
1:O:185:ARG:NH1	1:O:186:GLY:HA3	2.31	0.46
1:L:32:ASN:O	1:L:36:LYS:HG3	2.14	0.46
1:K:70:TYR:O	1:K:75:PHE:HB2	2.16	0.46
1:N:187:ILE:HD13	1:O:138:ASN:HB3	1.97	0.46
1:L:212:GLU:HG2	1:L:215:ARG:NH2	2.30	0.46
1:D:32:ASN:O	1:D:36:LYS:HG3	2.16	0.46
1:A:132:ILE:HB	1:A:166:LEU:HD21	1.97	0.46
1:L:185:ARG:HG2	1:L:186:GLY:N	2.31	0.46
1:O:159:LEU:O	1:O:163:GLN:HG3	2.15	0.46
1:L:101:VAL:HG21	1:L:137:ILE:HD12	1.98	0.46
1:H:19:LEU:HD21	1:I:93:MET:HA	1.97	0.45
1:A:185:ARG:NH1	1:A:186:GLY:HA3	2.31	0.45
1:J:185:ARG:NH1	1:J:186:GLY:HA3	2.31	0.45
1:J:32:ASN:O	1:J:36:LYS:HG3	2.16	0.45
1:C:32:ASN:O	1:C:36:LYS:HG3	2.17	0.45
1:A:192:SER:HA	1:B:102:ARG:O	2.17	0.45
1:L:187:ILE:HD13	1:M:138:ASN:HB3	1.98	0.45
1:A:139:ARG:HG2	1:E:187:ILE:HD12	1.99	0.45
1:B:135:SER:O	1:B:139:ARG:HG3	2.16	0.45
1:G:32:ASN:O	1:G:36:LYS:HG3	2.17	0.45
2:M:413:GTP:C2	1:N:134:LEU:HG	2.52	0.45
1:C:212:GLU:HG2	1:C:215:ARG:NH2	2.32	0.45
2:K:411:GTP:C2	1:L:134:LEU:HG	2.52	0.45
1:B:185:ARG:HG2	1:B:186:GLY:N	2.31	0.45
1:D:135:SER:O	1:D:139:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:32:ASN:O	1:N:36:LYS:HG3	2.17	0.45
1:L:208:ASN:O	1:L:212:GLU:HG3	2.17	0.45
1:A:32:ASN:O	1:A:36:LYS:HG3	2.17	0.45
2:B:402:GTP:C2	1:C:134:LEU:HG	2.51	0.45
1:J:208:ASN:O	1:J:212:GLU:HG3	2.17	0.45
1:I:185:ARG:HG2	1:I:186:GLY:N	2.33	0.44
1:C:187:ILE:HD13	1:D:138:ASN:HB3	1.98	0.44
1:B:187:ILE:HD12	1:C:139:ARG:HG2	1.98	0.44
1:D:212:GLU:HG2	1:D:215:ARG:NH2	2.32	0.44
1:K:212:GLU:HG2	1:K:215:ARG:NH2	2.32	0.44
1:O:32:ASN:O	1:O:36:LYS:HG3	2.17	0.44
1:A:185:ARG:HG2	1:A:186:GLY:N	2.33	0.44
1:I:13:ALA:O	1:I:17:ARG:HD3	2.17	0.44
1:D:159:LEU:O	1:D:163:GLN:HG3	2.18	0.44
1:O:155:THR:HG22	1:O:198:SER:OG	2.18	0.44
1:H:138:ASN:H	1:H:138:ASN:HD22	1.66	0.44
1:B:13:ALA:O	1:B:17:ARG:HD3	2.18	0.44
1:K:95:VAL:HG21	1:O:152:GLU:HB3	1.99	0.44
1:M:35:ARG:O	1:M:39:ILE:HG13	2.18	0.43
1:H:208:ASN:O	1:H:212:GLU:HG3	2.18	0.43
1:F:11:HIS:O	1:F:15:VAL:HG23	2.18	0.43
1:C:13:ALA:O	1:C:17:ARG:HD3	2.18	0.43
1:E:208:ASN:O	1:E:212:GLU:HG3	2.18	0.43
1:N:208:ASN:O	1:N:212:GLU:HG3	2.19	0.43
1:C:34:THR:O	1:C:38:LEU:HG	2.17	0.43
1:K:102:ARG:O	1:O:192:SER:HA	2.18	0.43
1:K:19:LEU:HD21	1:L:93:MET:HA	2.01	0.43
1:D:11:HIS:O	1:D:15:VAL:HG23	2.19	0.43
1:H:100:THR:HG23	1:H:124:ALA:HB2	1.98	0.43
1:G:192:SER:HA	1:H:102:ARG:O	2.18	0.43
1:H:185:ARG:HG2	1:H:186:GLY:N	2.34	0.43
1:J:13:ALA:O	1:J:17:ARG:HD3	2.19	0.43
1:I:155:THR:HG22	1:I:198:SER:OG	2.18	0.43
1:C:125:TYR:CD2	1:C:166:LEU:HD13	2.54	0.43
1:A:135:SER:O	1:A:139:ARG:HG3	2.18	0.43
1:B:11:HIS:O	1:B:15:VAL:HG23	2.19	0.43
1:L:138:ASN:HD22	1:L:138:ASN:H	1.66	0.43
1:M:159:LEU:O	1:M:163:GLN:HG3	2.19	0.43
1:B:125:TYR:CD2	1:B:166:LEU:HD13	2.54	0.43
1:B:208:ASN:O	1:B:212:GLU:HG3	2.19	0.42
1:H:212:GLU:HG2	1:H:215:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:75:PHE:CE1	1:M:148:PRO:HG3	2.54	0.42
1:J:155:THR:HG22	1:J:198:SER:OG	2.18	0.42
1:K:185:ARG:HH11	1:K:186:GLY:HA3	1.84	0.42
1:M:187:ILE:HD12	1:N:139:ARG:HG2	2.00	0.42
1:E:159:LEU:O	1:E:163:GLN:HG3	2.18	0.42
1:I:125:TYR:CD2	1:I:166:LEU:HD13	2.54	0.42
1:N:13:ALA:O	1:N:17:ARG:HD3	2.19	0.42
1:M:70:TYR:O	1:M:75:PHE:HB2	2.19	0.42
1:B:138:ASN:H	1:B:138:ASN:HD22	1.68	0.42
1:K:125:TYR:CD2	1:K:166:LEU:HD13	2.55	0.42
1:C:11:HIS:O	1:C:15:VAL:HG23	2.20	0.42
1:E:11:HIS:O	1:E:15:VAL:HG23	2.19	0.42
1:J:23:LEU:HD21	1:J:78:LEU:HD22	2.00	0.42
1:G:187:ILE:HD13	1:H:138:ASN:HB3	2.01	0.42
1:J:185:ARG:HG2	1:J:186:GLY:N	2.35	0.42
1:C:135:SER:O	1:C:139:ARG:HG3	2.20	0.42
1:N:192:SER:HA	1:O:102:ARG:O	2.20	0.42
1:E:138:ASN:HD22	1:E:138:ASN:H	1.66	0.42
2:G:407:GTP:C2	1:H:134:LEU:HG	2.54	0.42
1:I:187:ILE:HD13	1:J:138:ASN:HB3	2.02	0.42
1:H:135:SER:O	1:H:139:ARG:HG3	2.19	0.41
1:M:185:ARG:HH11	1:M:186:GLY:HA3	1.83	0.41
1:A:138:ASN:CB	1:E:187:ILE:HD13	2.50	0.41
1:K:138:ASN:HB3	1:O:187:ILE:HD13	2.03	0.41
1:M:212:GLU:HG2	1:M:215:ARG:NH2	2.35	0.41
1:G:13:ALA:O	1:G:17:ARG:HD3	2.21	0.41
1:B:19:LEU:CD2	1:C:93:MET:HA	2.50	0.41
1:C:155:THR:HG22	1:C:198:SER:OG	2.19	0.41
1:H:11:HIS:O	1:H:15:VAL:HG23	2.21	0.41
1:O:135:SER:O	1:O:139:ARG:HG3	2.20	0.41
1:G:100:THR:HG23	1:G:124:ALA:HB2	2.02	0.41
1:A:102:ARG:O	1:E:192:SER:HA	2.21	0.41
1:M:208:ASN:O	1:M:212:GLU:HG3	2.20	0.41
1:A:208:ASN:O	1:A:212:GLU:HG3	2.20	0.41
1:A:13:ALA:O	1:A:17:ARG:HD3	2.21	0.41
1:L:155:THR:HG22	1:L:198:SER:OG	2.20	0.41
1:I:208:ASN:O	1:I:212:GLU:HG3	2.21	0.41
1:J:212:GLU:HG2	1:J:215:ARG:NH2	2.36	0.41
1:M:11:HIS:O	1:M:15:VAL:HG23	2.21	0.41
1:F:13:ALA:O	1:F:17:ARG:HD3	2.21	0.40
1:N:137:ILE:O	1:N:141:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:O	1:C:124:ALA:HA	2.21	0.40
1:C:208:ASN:O	1:C:212:GLU:HG3	2.21	0.40
1:C:187:ILE:HD12	1:D:139:ARG:HG2	2.02	0.40
1:H:70:TYR:O	1:H:75:PHE:HB2	2.21	0.40
1:H:19:LEU:HD13	1:H:156:GLN:HB3	2.04	0.40
1:K:19:LEU:HA	1:K:19:LEU:HD23	1.96	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	219/221 (99%)	207 (94%)	8 (4%)	4 (2%)	11	37
1	B	219/221 (99%)	208 (95%)	6 (3%)	5 (2%)	8	30
1	C	219/221 (99%)	206 (94%)	8 (4%)	5 (2%)	8	30
1	D	219/221 (99%)	203 (93%)	11 (5%)	5 (2%)	8	30
1	E	219/221 (99%)	204 (93%)	11 (5%)	4 (2%)	11	37
1	F	219/221 (99%)	206 (94%)	8 (4%)	5 (2%)	8	30
1	G	219/221 (99%)	206 (94%)	8 (4%)	5 (2%)	8	30
1	H	219/221 (99%)	205 (94%)	9 (4%)	5 (2%)	8	30
1	I	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	11	37
1	J	219/221 (99%)	204 (93%)	10 (5%)	5 (2%)	8	30
1	K	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	11	37
1	L	219/221 (99%)	207 (94%)	7 (3%)	5 (2%)	8	30
1	M	219/221 (99%)	207 (94%)	8 (4%)	4 (2%)	11	37
1	N	219/221 (99%)	204 (93%)	10 (5%)	5 (2%)	8	30
1	O	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	11	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3285/3315 (99%)	3076 (94%)	140 (4%)	69 (2%)	9	32

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	C	2	SER
1	D	2	SER
1	E	2	SER
1	J	2	SER
1	K	2	SER
1	L	2	SER
1	M	2	SER
1	N	2	SER
1	B	2	SER
1	D	26	PRO
1	F	2	SER
1	G	2	SER
1	H	2	SER
1	I	2	SER
1	K	26	PRO
1	N	26	PRO
1	O	2	SER
1	A	26	PRO
1	B	26	PRO
1	C	26	PRO
1	E	26	PRO
1	F	26	PRO
1	G	26	PRO
1	H	26	PRO
1	I	26	PRO
1	J	26	PRO
1	L	26	PRO
1	M	26	PRO
1	O	26	PRO
1	B	218	ARG
1	C	218	ARG
1	D	218	ARG
1	F	218	ARG
1	G	218	ARG
1	K	218	ARG
1	L	218	ARG

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Mol	Chain	Res	Type
1	N	218	ARG
1	C	22	PRO
1	D	27	VAL
1	E	218	ARG
1	G	22	PRO
1	H	218	ARG
1	I	218	ARG
1	J	218	ARG
1	M	22	PRO
1	M	218	ARG
1	A	22	PRO
1	F	22	PRO
1	J	22	PRO
1	J	27	VAL
1	L	22	PRO
1	B	22	PRO
1	B	27	VAL
1	C	27	VAL
1	E	22	PRO
1	H	22	PRO
1	K	27	VAL
1	N	22	PRO
1	O	22	PRO
1	A	27	VAL
1	D	22	PRO
1	F	27	VAL
1	G	27	VAL
1	H	27	VAL
1	I	27	VAL
1	L	27	VAL
1	N	27	VAL
1	O	27	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	B	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	C	194/194 (100%)	191 (98%)	3 (2%)	72	92
1	D	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	E	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	F	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	G	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	H	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	I	194/194 (100%)	191 (98%)	3 (2%)	72	92
1	J	194/194 (100%)	191 (98%)	3 (2%)	72	92
1	K	194/194 (100%)	191 (98%)	3 (2%)	72	92
1	L	194/194 (100%)	191 (98%)	3 (2%)	72	92
1	M	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	N	194/194 (100%)	190 (98%)	4 (2%)	61	88
1	O	194/194 (100%)	190 (98%)	4 (2%)	61	88
All	All	2910/2910 (100%)	2855 (98%)	55 (2%)	65	89

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	93	MET
1	A	168	THR
1	A	185	ARG
1	B	20	GLU
1	B	93	MET
1	B	168	THR
1	B	185	ARG
1	C	20	GLU
1	C	93	MET
1	C	185	ARG
1	D	20	GLU
1	D	93	MET
1	D	168	THR
1	D	185	ARG
1	E	20	GLU
1	E	93	MET
1	E	168	THR

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Mol	Chain	Res	Type
1	E	185	ARG
1	F	20	GLU
1	F	93	MET
1	F	168	THR
1	F	185	ARG
1	G	20	GLU
1	G	93	MET
1	G	168	THR
1	G	185	ARG
1	H	20	GLU
1	H	93	MET
1	H	168	THR
1	H	185	ARG
1	I	20	GLU
1	I	93	MET
1	I	185	ARG
1	J	20	GLU
1	J	93	MET
1	J	185	ARG
1	K	20	GLU
1	K	93	MET
1	K	185	ARG
1	L	20	GLU
1	L	93	MET
1	L	185	ARG
1	M	20	GLU
1	M	93	MET
1	M	168	THR
1	M	185	ARG
1	N	20	GLU
1	N	93	MET
1	N	168	THR
1	N	185	ARG
1	O	20	GLU
1	O	93	MET
1	O	168	THR
1	O	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	163	GLN
1	D	138	ASN
1	E	138	ASN
1	E	163	GLN
1	G	138	ASN
1	H	138	ASN
1	H	163	GLN
1	K	138	ASN
1	L	138	ASN
1	L	163	GLN
1	M	138	ASN
1	N	138	ASN
1	O	138	ASN
1	O	163	GLN

### 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 ⓘ

15 ligands are 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	GTP	A	401	-	25,34,34	1.34	3 (12%)	34,54,54	2.44	11 (32%)
2	GTP	B	402	-	25,34,34	1.40	4 (16%)	34,54,54	2.46	9 (26%)
2	GTP	C	403	-	25,34,34	1.44	4 (16%)	34,54,54	2.45	12 (35%)
2	GTP	D	404	-	25,34,34	1.28	2 (8%)	34,54,54	2.46	12 (35%)
2	GTP	E	405	-	25,34,34	1.38	3 (12%)	34,54,54	2.53	13 (38%)
2	GTP	F	406	-	25,34,34	1.42	3 (12%)	34,54,54	2.44	11 (32%)
2	GTP	G	407	-	25,34,34	1.33	3 (12%)	34,54,54	2.53	14 (41%)
2	GTP	H	408	-	25,34,34	1.38	3 (12%)	34,54,54	2.40	12 (35%)
2	GTP	I	409	-	25,34,34	1.44	6 (24%)	34,54,54	2.46	13 (38%)
2	GTP	J	410	-	25,34,34	1.27	2 (8%)	34,54,54	2.45	13 (38%)
2	GTP	K	411	-	25,34,34	1.38	5 (20%)	34,54,54	2.46	12 (35%)
2	GTP	L	412	-	25,34,34	1.35	4 (16%)	34,54,54	2.49	12 (35%)
2	GTP	M	413	-	25,34,34	1.36	3 (12%)	34,54,54	2.42	9 (26%)
2	GTP	N	414	-	25,34,34	1.32	4 (16%)	34,54,54	2.44	12 (35%)
2	GTP	O	415	-	25,34,34	1.47	5 (20%)	34,54,54	2.47	11 (32%)

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	-	-	0/18/38/38	0/3/3/3
2	GTP	B	402	-	-	0/18/38/38	0/3/3/3
2	GTP	C	403	-	-	0/18/38/38	0/3/3/3
2	GTP	D	404	-	-	0/18/38/38	0/3/3/3
2	GTP	E	405	-	-	0/18/38/38	0/3/3/3
2	GTP	F	406	-	-	0/18/38/38	0/3/3/3
2	GTP	G	407	-	-	0/18/38/38	0/3/3/3
2	GTP	H	408	-	-	0/18/38/38	0/3/3/3
2	GTP	I	409	-	-	0/18/38/38	0/3/3/3
2	GTP	J	410	-	-	0/18/38/38	0/3/3/3
2	GTP	K	411	-	-	0/18/38/38	0/3/3/3
2	GTP	L	412	-	-	0/18/38/38	0/3/3/3
2	GTP	M	413	-	-	0/18/38/38	0/3/3/3
2	GTP	N	414	-	-	0/18/38/38	0/3/3/3
2	GTP	O	415	-	-	0/18/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	409	GTP	O6-C6	-2.34	1.19	1.24
2	M	413	GTP	PB-O2B	-2.28	1.45	1.54
2	B	402	GTP	O6-C6	-2.19	1.19	1.24
2	K	411	GTP	O6-C6	-2.16	1.19	1.24
2	N	414	GTP	O6-C6	-2.13	1.19	1.24
2	O	415	GTP	PB-O2B	-2.07	1.46	1.54
2	J	410	GTP	O6-C6	-2.06	1.19	1.24
2	G	407	GTP	O6-C6	-2.05	1.19	1.24
2	L	412	GTP	O6-C6	-2.04	1.19	1.24
2	L	412	GTP	C5-C4	-2.03	1.35	1.40
2	I	409	GTP	PB-O2B	-2.00	1.46	1.54
2	O	415	GTP	O2'-C2'	2.01	1.47	1.43
2	C	403	GTP	PG-O3G	2.02	1.62	1.54
2	O	415	GTP	O4'-C4'	2.02	1.49	1.45
2	B	402	GTP	O2'-C2'	2.06	1.47	1.43
2	B	402	GTP	PG-O3G	2.07	1.62	1.54
2	J	410	GTP	O4'-C4'	2.09	1.49	1.45
2	N	414	GTP	O2'-C2'	2.11	1.48	1.43
2	I	409	GTP	PG-O3G	2.12	1.62	1.54
2	E	405	GTP	O2'-C2'	2.13	1.48	1.43
2	K	411	GTP	O2'-C2'	2.14	1.48	1.43
2	A	401	GTP	O2'-C2'	2.15	1.48	1.43
2	C	403	GTP	O2'-C2'	2.16	1.48	1.43
2	E	405	GTP	C2-N1	2.16	1.39	1.35
2	H	408	GTP	O2'-C2'	2.18	1.48	1.43
2	D	404	GTP	O2'-C2'	2.19	1.48	1.43
2	F	406	GTP	O2'-C2'	2.26	1.48	1.43
2	I	409	GTP	O4'-C4'	2.34	1.50	1.45
2	K	411	GTP	O4'-C4'	2.38	1.50	1.45
2	N	414	GTP	C2-N1	2.40	1.39	1.35
2	K	411	GTP	C2-N1	2.40	1.39	1.35
2	L	412	GTP	O4'-C4'	2.42	1.50	1.45
2	I	409	GTP	C2-N1	2.45	1.39	1.35
2	L	412	GTP	C6-N1	2.46	1.37	1.33
2	A	401	GTP	C2-N1	2.46	1.39	1.35
2	I	409	GTP	C6-N1	2.51	1.37	1.33
2	M	413	GTP	C2-N1	2.53	1.39	1.35
2	F	406	GTP	C2-N1	2.63	1.40	1.35
2	C	403	GTP	C2-N1	2.64	1.40	1.35
2	B	402	GTP	C6-N1	2.67	1.38	1.33
2	G	407	GTP	C2-N1	2.68	1.40	1.35
2	K	411	GTP	C6-N1	2.69	1.38	1.33
2	G	407	GTP	C6-N1	2.89	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	404	GTP	C6-N1	2.90	1.38	1.33
2	N	414	GTP	C6-N1	3.03	1.38	1.33
2	M	413	GTP	C6-N1	3.06	1.38	1.33
2	O	415	GTP	C2-N1	3.07	1.40	1.35
2	H	408	GTP	C2-N1	3.07	1.40	1.35
2	A	401	GTP	C6-N1	3.10	1.38	1.33
2	C	403	GTP	C6-N1	3.22	1.39	1.33
2	F	406	GTP	C6-N1	3.48	1.39	1.33
2	H	408	GTP	C6-N1	3.50	1.39	1.33
2	E	405	GTP	C6-N1	3.58	1.39	1.33
2	O	415	GTP	C6-N1	3.70	1.40	1.33

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GTP	C5-C6-N1	-7.65	113.13	123.59
2	O	415	GTP	C5-C6-N1	-7.58	113.22	123.59
2	F	406	GTP	C5-C6-N1	-7.56	113.25	123.59
2	D	404	GTP	C5-C6-N1	-7.52	113.31	123.59
2	G	407	GTP	C5-C6-N1	-7.49	113.35	123.59
2	E	405	GTP	C5-C6-N1	-7.45	113.40	123.59
2	M	413	GTP	C5-C6-N1	-7.45	113.41	123.59
2	B	402	GTP	C5-C6-N1	-7.43	113.43	123.59
2	C	403	GTP	C5-C6-N1	-7.42	113.44	123.59
2	L	412	GTP	C5-C6-N1	-7.41	113.46	123.59
2	I	409	GTP	C5-C6-N1	-7.39	113.49	123.59
2	J	410	GTP	C5-C6-N1	-7.33	113.57	123.59
2	H	408	GTP	C5-C6-N1	-7.32	113.58	123.59
2	K	411	GTP	C5-C6-N1	-7.32	113.58	123.59
2	N	414	GTP	C5-C6-N1	-7.22	113.71	123.59
2	L	412	GTP	C4'-O4'-C1'	-5.85	103.29	109.72
2	E	405	GTP	C4'-O4'-C1'	-5.45	103.73	109.72
2	G	407	GTP	C4'-O4'-C1'	-5.44	103.74	109.72
2	K	411	GTP	C4'-O4'-C1'	-5.42	103.76	109.72
2	A	401	GTP	C4'-O4'-C1'	-5.23	103.97	109.72
2	B	402	GTP	C4'-O4'-C1'	-5.20	104.01	109.72
2	M	413	GTP	C4'-O4'-C1'	-5.11	104.10	109.72
2	H	408	GTP	C4'-O4'-C1'	-5.00	104.22	109.72
2	D	404	GTP	C4'-O4'-C1'	-5.00	104.23	109.72
2	N	414	GTP	C4'-O4'-C1'	-4.99	104.23	109.72
2	J	410	GTP	C4'-O4'-C1'	-4.72	104.53	109.72
2	C	403	GTP	C4'-O4'-C1'	-4.72	104.53	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	409	GTP	C4'-O4'-C1'	-4.71	104.55	109.72
2	O	415	GTP	C4'-O4'-C1'	-4.71	104.55	109.72
2	F	406	GTP	C4'-O4'-C1'	-4.59	104.68	109.72
2	N	414	GTP	N3-C2-N1	-3.87	121.55	127.44
2	C	403	GTP	N3-C2-N1	-3.71	121.80	127.44
2	O	415	GTP	N3-C2-N1	-3.70	121.81	127.44
2	I	409	GTP	N3-C2-N1	-3.64	121.91	127.44
2	E	405	GTP	N3-C2-N1	-3.63	121.91	127.44
2	B	402	GTP	N3-C2-N1	-3.60	121.96	127.44
2	G	407	GTP	N3-C2-N1	-3.60	121.97	127.44
2	D	404	GTP	N3-C2-N1	-3.54	122.05	127.44
2	F	406	GTP	N3-C2-N1	-3.44	122.20	127.44
2	K	411	GTP	N3-C2-N1	-3.44	122.20	127.44
2	H	408	GTP	N3-C2-N1	-3.43	122.22	127.44
2	L	412	GTP	N3-C2-N1	-3.33	122.36	127.44
2	L	412	GTP	PB-O3B-PG	-3.26	121.75	132.67
2	M	413	GTP	N3-C2-N1	-3.24	122.51	127.44
2	J	410	GTP	N3-C2-N1	-3.22	122.55	127.44
2	A	401	GTP	N3-C2-N1	-3.16	122.64	127.44
2	G	407	GTP	PB-O3B-PG	-2.95	122.78	132.67
2	E	405	GTP	C5'-C4'-C3'	-2.95	103.52	115.21
2	M	413	GTP	PB-O3B-PG	-2.93	122.84	132.67
2	J	410	GTP	C5'-C4'-C3'	-2.87	103.81	115.21
2	J	410	GTP	PB-O3B-PG	-2.85	123.09	132.67
2	B	402	GTP	C5'-C4'-C3'	-2.83	103.98	115.21
2	L	412	GTP	C5'-C4'-C3'	-2.82	104.00	115.21
2	M	413	GTP	C5'-C4'-C3'	-2.81	104.06	115.21
2	G	407	GTP	C5'-C4'-C3'	-2.81	104.06	115.21
2	D	404	GTP	C5'-C4'-C3'	-2.79	104.13	115.21
2	O	415	GTP	PB-O3B-PG	-2.75	123.46	132.67
2	K	411	GTP	C5'-C4'-C3'	-2.72	104.40	115.21
2	C	403	GTP	PB-O3B-PG	-2.72	123.55	132.67
2	F	406	GTP	PB-O3B-PG	-2.72	123.56	132.67
2	I	409	GTP	C5'-C4'-C3'	-2.71	104.44	115.21
2	N	414	GTP	C5'-C4'-C3'	-2.71	104.45	115.21
2	D	404	GTP	PB-O3B-PG	-2.70	123.61	132.67
2	C	403	GTP	C5'-C4'-C3'	-2.69	104.53	115.21
2	A	401	GTP	C5'-C4'-C3'	-2.69	104.55	115.21
2	F	406	GTP	C5'-C4'-C3'	-2.66	104.67	115.21
2	O	415	GTP	C5'-C4'-C3'	-2.64	104.72	115.21
2	H	408	GTP	C5'-C4'-C3'	-2.64	104.74	115.21
2	B	402	GTP	PB-O3B-PG	-2.60	123.95	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	405	GTP	PB-O3B-PG	-2.48	124.36	132.67
2	H	408	GTP	PB-O3B-PG	-2.47	124.39	132.67
2	G	407	GTP	O5'-PA-O1A	-2.38	100.39	109.62
2	K	411	GTP	PB-O3B-PG	-2.38	124.70	132.67
2	C	403	GTP	O5'-PA-O1A	-2.34	100.52	109.62
2	L	412	GTP	O5'-PA-O1A	-2.34	100.55	109.62
2	O	415	GTP	C1'-N9-C4	-2.33	123.43	126.94
2	H	408	GTP	C1'-N9-C4	-2.32	123.44	126.94
2	J	410	GTP	O5'-PA-O1A	-2.32	100.62	109.62
2	I	409	GTP	PB-O3B-PG	-2.31	124.93	132.67
2	N	414	GTP	PB-O3B-PG	-2.30	124.94	132.67
2	J	410	GTP	O5'-C5'-C4'	-2.28	100.72	109.12
2	E	405	GTP	C1'-N9-C4	-2.25	123.55	126.94
2	A	401	GTP	PB-O3B-PG	-2.25	125.13	132.67
2	I	409	GTP	C1'-N9-C4	-2.24	123.56	126.94
2	E	405	GTP	C6-C5-C4	-2.21	118.25	120.90
2	E	405	GTP	O5'-PA-O1A	-2.21	101.02	109.62
2	J	410	GTP	C6-C5-C4	-2.18	118.29	120.90
2	F	406	GTP	C1'-N9-C4	-2.17	123.67	126.94
2	L	412	GTP	O5'-C5'-C4'	-2.17	101.14	109.12
2	H	408	GTP	O5'-PA-O1A	-2.15	101.27	109.62
2	G	407	GTP	O5'-C5'-C4'	-2.15	101.19	109.12
2	O	415	GTP	O5'-PA-O1A	-2.13	101.33	109.62
2	N	414	GTP	C1'-N9-C4	-2.11	123.75	126.94
2	E	405	GTP	O5'-C5'-C4'	-2.11	101.34	109.12
2	A	401	GTP	C6-C5-C4	-2.09	118.40	120.90
2	K	411	GTP	C6-C5-C4	-2.08	118.41	120.90
2	I	409	GTP	C6-C5-C4	-2.05	118.44	120.90
2	K	411	GTP	C1'-N9-C4	-2.05	123.84	126.94
2	A	401	GTP	O5'-C5'-C4'	-2.05	101.55	109.12
2	G	407	GTP	C1'-N9-C4	-2.04	123.86	126.94
2	N	414	GTP	O5'-C5'-C4'	-2.04	101.58	109.12
2	J	410	GTP	C1'-N9-C4	-2.04	123.87	126.94
2	G	407	GTP	C6-C5-C4	-2.03	118.47	120.90
2	D	404	GTP	O5'-PA-O1A	-2.03	101.75	109.62
2	I	409	GTP	O5'-C5'-C4'	-2.02	101.67	109.12
2	D	404	GTP	O5'-C5'-C4'	-2.02	101.69	109.12
2	N	414	GTP	O5'-PA-O1A	-2.01	101.82	109.62
2	L	412	GTP	O2'-C2'-C3'	2.02	118.39	111.83
2	I	409	GTP	O2'-C2'-C3'	2.02	118.40	111.83
2	J	410	GTP	O2A-PA-O3A	2.04	114.35	105.09
2	G	407	GTP	O2A-PA-O3A	2.06	114.45	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	GTP	O2'-C2'-C3'	2.07	118.54	111.83
2	G	407	GTP	O2'-C2'-C3'	2.08	118.59	111.83
2	C	403	GTP	O2B-PB-O3B	2.09	114.57	105.09
2	H	408	GTP	O2'-C2'-C3'	2.11	118.68	111.83
2	F	406	GTP	O2A-PA-O3A	2.11	114.67	105.09
2	H	408	GTP	O2A-PA-O3A	2.15	114.85	105.09
2	C	403	GTP	O2'-C2'-C3'	2.15	118.83	111.83
2	N	414	GTP	O2A-PA-O3A	2.15	114.86	105.09
2	K	411	GTP	O2'-C2'-C3'	2.15	118.83	111.83
2	F	406	GTP	O2'-C2'-C3'	2.18	118.92	111.83
2	K	411	GTP	O2A-PA-O3A	2.20	115.05	105.09
2	E	405	GTP	O2A-PA-O3A	2.20	115.08	105.09
2	D	404	GTP	O2A-PA-O3A	2.20	115.08	105.09
2	M	413	GTP	O2A-PA-O3A	2.20	115.09	105.09
2	A	401	GTP	O2A-PA-O3A	2.23	115.20	105.09
2	O	415	GTP	O2A-PA-O3A	2.23	115.21	105.09
2	C	403	GTP	O2A-PA-O3A	2.25	115.29	105.09
2	D	404	GTP	O2'-C2'-C3'	2.25	119.16	111.83
2	M	413	GTP	O2G-PG-O1G	2.28	117.92	110.58
2	I	409	GTP	O2A-PA-O3A	2.28	115.43	105.09
2	L	412	GTP	O2A-PA-O3A	2.28	115.44	105.09
2	A	401	GTP	O2G-PG-O1G	2.36	118.19	110.58
2	L	412	GTP	O2G-PG-O1G	2.41	118.33	110.58
2	K	411	GTP	O2G-PG-O1G	2.48	118.55	110.58
2	J	410	GTP	O2G-PG-O1G	2.52	118.70	110.58
2	I	409	GTP	O2G-PG-O1G	2.55	118.79	110.58
2	N	414	GTP	O2G-PG-O1G	2.60	118.95	110.58
2	B	402	GTP	O2G-PG-O1G	2.61	118.97	110.58
2	H	408	GTP	O2G-PG-O1G	2.62	119.00	110.58
2	D	404	GTP	O2G-PG-O1G	2.62	119.02	110.58
2	C	403	GTP	O2G-PG-O1G	2.68	119.21	110.58
2	O	415	GTP	O2G-PG-O1G	2.68	119.21	110.58
2	F	406	GTP	O2G-PG-O1G	2.71	119.29	110.58
2	G	407	GTP	O2G-PG-O1G	2.74	119.40	110.58
2	E	405	GTP	O2G-PG-O1G	2.83	119.69	110.58
2	C	403	GTP	O4'-C4'-C5'	2.83	119.45	109.32
2	A	401	GTP	O4'-C4'-C5'	2.86	119.55	109.32
2	O	415	GTP	O4'-C4'-C5'	2.88	119.61	109.32
2	N	414	GTP	O4'-C4'-C5'	2.88	119.61	109.32
2	G	407	GTP	O4'-C4'-C5'	2.89	119.65	109.32
2	I	409	GTP	O4'-C4'-C5'	2.91	119.72	109.32
2	J	410	GTP	O4'-C4'-C5'	2.91	119.73	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	413	GTP	O4'-C4'-C5'	2.93	119.79	109.32
2	D	404	GTP	O4'-C4'-C5'	2.93	119.80	109.32
2	H	408	GTP	O4'-C4'-C5'	2.98	119.98	109.32
2	F	406	GTP	O4'-C4'-C5'	3.00	120.05	109.32
2	L	412	GTP	O4'-C4'-C5'	3.02	120.11	109.32
2	K	411	GTP	O4'-C4'-C5'	3.02	120.12	109.32
2	B	402	GTP	O4'-C4'-C5'	3.04	120.18	109.32
2	E	405	GTP	O4'-C4'-C5'	3.06	120.28	109.32
2	H	408	GTP	C6-N1-C2	5.74	123.91	115.94
2	L	412	GTP	C6-N1-C2	5.78	123.96	115.94
2	M	413	GTP	C6-N1-C2	5.84	124.04	115.94
2	F	406	GTP	C6-N1-C2	5.90	124.13	115.94
2	C	403	GTP	C6-N1-C2	5.95	124.20	115.94
2	A	401	GTP	C6-N1-C2	5.95	124.20	115.94
2	D	404	GTP	C6-N1-C2	5.96	124.21	115.94
2	N	414	GTP	C6-N1-C2	5.98	124.25	115.94
2	I	409	GTP	C6-N1-C2	6.00	124.27	115.94
2	B	402	GTP	C6-N1-C2	6.03	124.31	115.94
2	E	405	GTP	C6-N1-C2	6.06	124.35	115.94
2	O	415	GTP	C6-N1-C2	6.06	124.36	115.94
2	J	410	GTP	C6-N1-C2	6.10	124.40	115.94
2	K	411	GTP	C6-N1-C2	6.10	124.41	115.94
2	G	407	GTP	C6-N1-C2	6.13	124.45	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	GTP	1	0
2	C	403	GTP	1	0
2	G	407	GTP	1	0
2	I	409	GTP	1	0
2	J	410	GTP	1	0
2	K	411	GTP	1	0
2	M	413	GTP	1	0
2	N	414	GTP	1	0
2	O	415	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.