



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:46 AM GMT

PDB ID : 1A8R  
Title : GTP CYCLOHYDROLASE I (H112S MUTANT) IN COMPLEX WITH GTP  
Authors : Auerbach, G.; Nar, H.; Bracher, A.; Bacher, A.; Huber, R.  
Deposited on : 1998-03-27  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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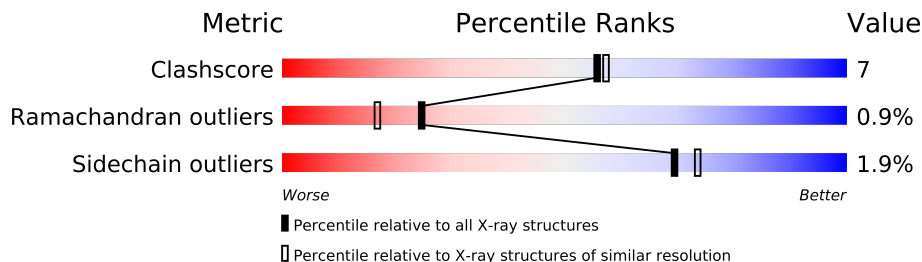
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.









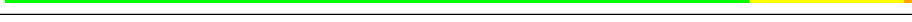

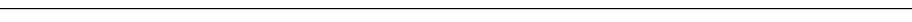
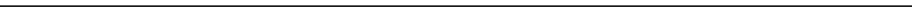


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	
1	H	221	
1	I	221	
1	J	221	
1	K	221	
1	L	221	
1	M	221	
1	N	221	
1	O	221	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27375 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

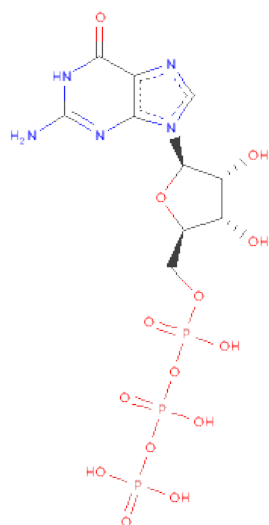
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	B	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	C	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	D	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	E	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	F	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	G	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	H	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	I	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	J	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	K	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	L	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	M	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	N	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	O	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	SER	HIS	MUTATION	UNP P0A6T5
B	112	SER	HIS	MUTATION	UNP P0A6T5
C	112	SER	HIS	MUTATION	UNP P0A6T5
D	112	SER	HIS	MUTATION	UNP P0A6T5
E	112	SER	HIS	MUTATION	UNP P0A6T5
F	112	SER	HIS	MUTATION	UNP P0A6T5
G	112	SER	HIS	MUTATION	UNP P0A6T5
H	112	SER	HIS	MUTATION	UNP P0A6T5
I	112	SER	HIS	MUTATION	UNP P0A6T5
J	112	SER	HIS	MUTATION	UNP P0A6T5
K	112	SER	HIS	MUTATION	UNP P0A6T5
L	112	SER	HIS	MUTATION	UNP P0A6T5
M	112	SER	HIS	MUTATION	UNP P0A6T5
N	112	SER	HIS	MUTATION	UNP P0A6T5
O	112	SER	HIS	MUTATION	UNP P0A6T5

- 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	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	66	Total	O	0	0
			66	66		
3	B	64	Total	O	0	0
			64	64		
3	C	66	Total	O	0	0
			66	66		
3	D	66	Total	O	0	0
			66	66		
3	E	63	Total	O	0	0
			63	63		
3	F	66	Total	O	0	0
			66	66		
3	G	67	Total	O	0	0
			67	67		
3	H	64	Total	O	0	0
			64	64		

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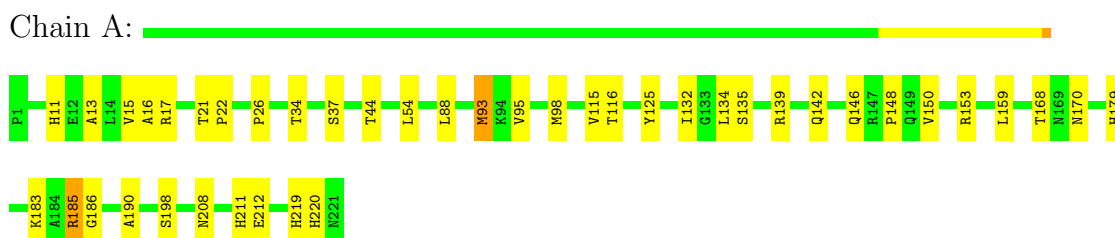
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	67	Total 67	O 67	0	0
3	J	61	Total 61	O 61	0	0
3	K	65	Total 65	O 65	0	0
3	L	65	Total 65	O 65	0	0
3	M	68	Total 68	O 68	0	0
3	N	64	Total 64	O 64	0	0
3	O	63	Total 63	O 63	0	0

### 3 Residue-property plots

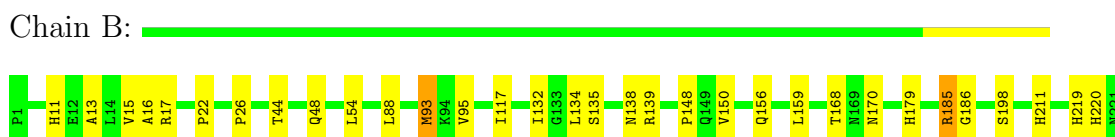
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

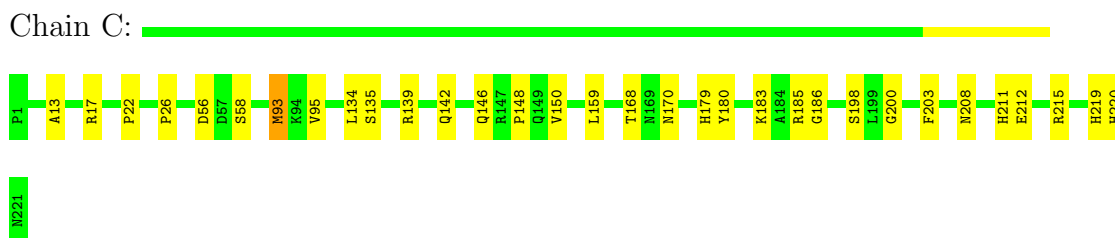
#### • Molecule 1: GTP CYCLOHYDROLASE I



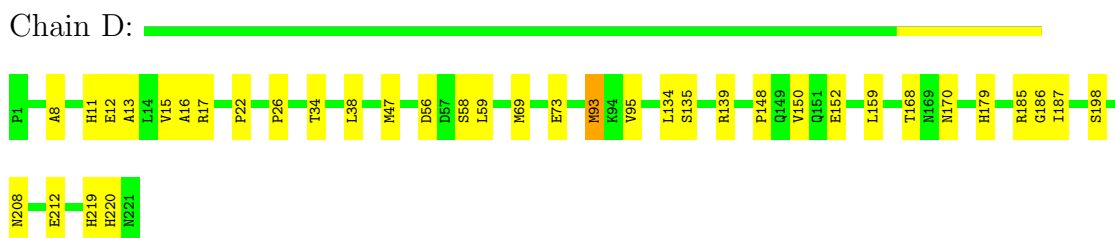
#### • Molecule 1: GTP CYCLOHYDROLASE I



#### • Molecule 1: GTP CYCLOHYDROLASE I

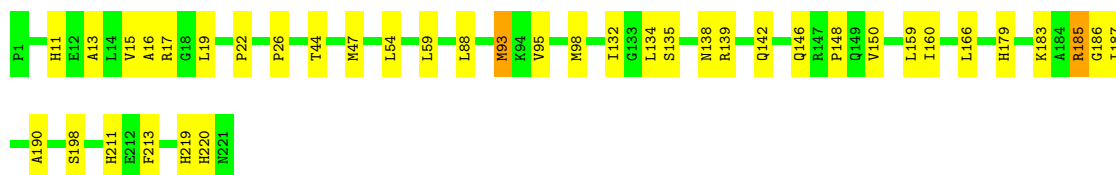


#### • Molecule 1: GTP CYCLOHYDROLASE I



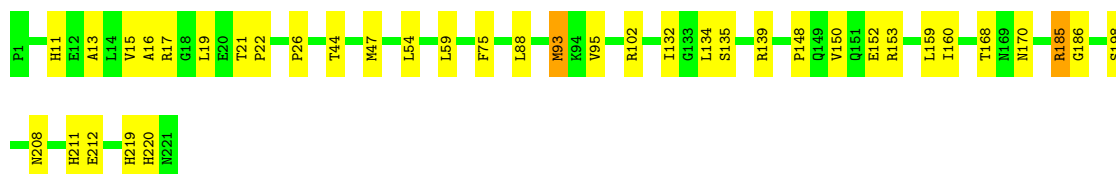
#### • Molecule 1: GTP CYCLOHYDROLASE I





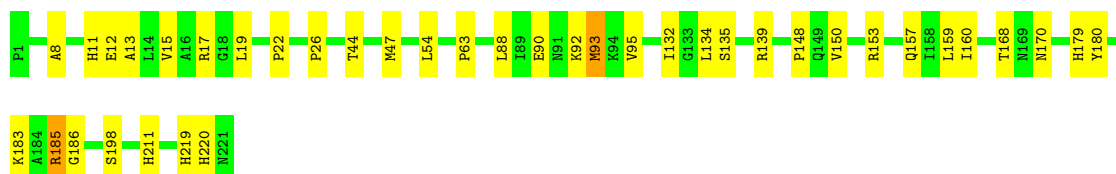
• Molecule 1: GTP CYCLOHYDROLASE I

Chain F:



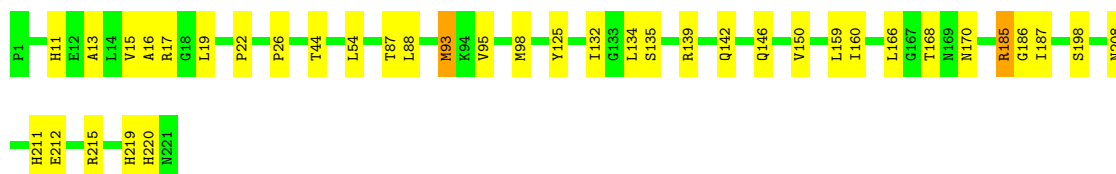
• Molecule 1: GTP CYCLOHYDROLASE I

Chain G:



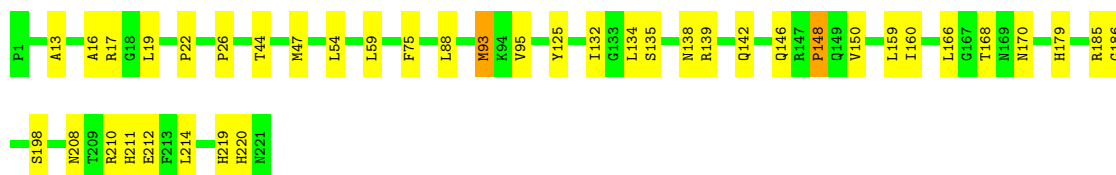
• Molecule 1: GTP CYCLOHYDROLASE I

Chain H:



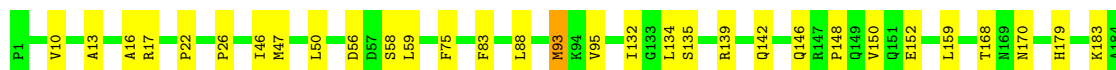
• Molecule 1: GTP CYCLOHYDROLASE I

Chain I:



• Molecule 1: GTP CYCLOHYDROLASE I

Chain J:

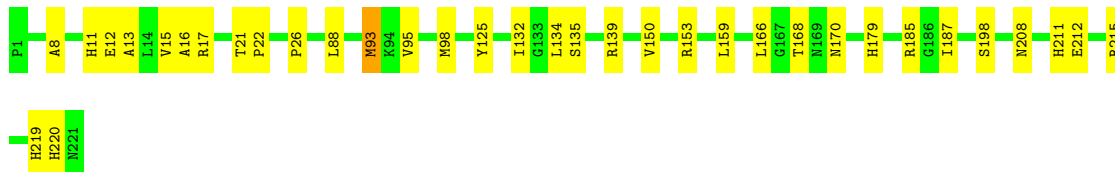






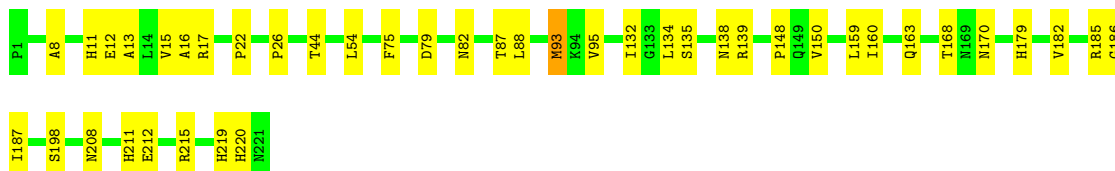
• Molecule 1: GTP CYCLOHYDROLASE I

Chain K:



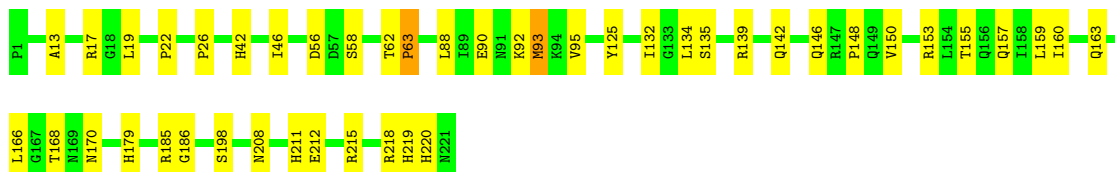
• Molecule 1: GTP CYCLOHYDROLASE I

Chain L:



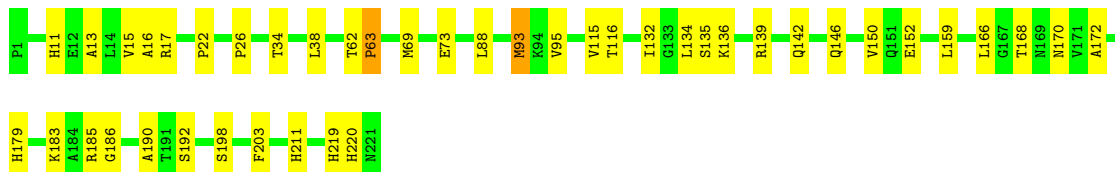
• Molecule 1: GTP CYCLOHYDROLASE I

Chain M:



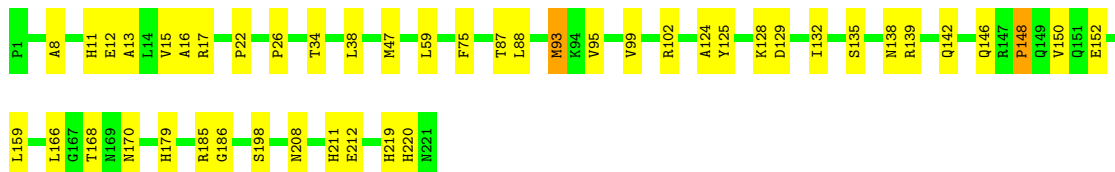
• Molecule 1: GTP CYCLOHYDROLASE I

Chain N:



• Molecule 1: GTP CYCLOHYDROLASE I

Chain O:



## 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, $\alpha$ , $\beta$ , $\gamma$	314.95Å 219.14Å 131.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.4 (8.00-2.10)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.200 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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	0.52	0/1755	0.82	2/2377 (0.1%)
1	B	0.53	0/1755	0.82	3/2377 (0.1%)
1	C	0.53	0/1755	0.82	2/2377 (0.1%)
1	D	0.53	0/1755	0.82	2/2377 (0.1%)
1	E	0.51	0/1755	0.79	2/2377 (0.1%)
1	F	0.50	0/1755	0.77	1/2377 (0.0%)
1	G	0.50	0/1755	0.79	2/2377 (0.1%)
1	H	0.51	0/1755	0.81	1/2377 (0.0%)
1	I	0.52	0/1755	0.80	2/2377 (0.1%)
1	J	0.54	0/1755	0.81	1/2377 (0.0%)
1	K	0.53	0/1755	0.82	1/2377 (0.0%)
1	L	0.49	0/1755	0.79	1/2377 (0.0%)
1	M	0.51	0/1755	0.81	2/2377 (0.1%)
1	N	0.52	0/1755	0.80	1/2377 (0.0%)
1	O	0.50	0/1755	0.79	2/2377 (0.1%)
All	All	0.52	0/26325	0.80	25/35655 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	150	VAL	N-CA-C	-6.28	94.05	111.00
1	C	150	VAL	N-CA-C	-6.25	94.12	111.00
1	D	150	VAL	N-CA-C	-6.23	94.19	111.00
1	H	150	VAL	N-CA-C	-6.16	94.36	111.00
1	K	150	VAL	N-CA-C	-6.15	94.40	111.00
1	G	150	VAL	N-CA-C	-6.11	94.50	111.00
1	B	150	VAL	N-CA-C	-6.02	94.75	111.00
1	M	150	VAL	N-CA-C	-6.02	94.75	111.00
1	O	150	VAL	N-CA-C	-5.93	94.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	150	VAL	N-CA-C	-5.86	95.17	111.00
1	A	150	VAL	N-CA-C	-5.83	95.27	111.00
1	N	150	VAL	N-CA-C	-5.77	95.41	111.00
1	D	148	PRO	N-CA-C	-5.67	97.35	112.10
1	M	148	PRO	N-CA-C	-5.59	97.56	112.10
1	C	148	PRO	N-CA-C	-5.57	97.63	112.10
1	I	150	VAL	N-CA-C	-5.54	96.06	111.00
1	L	150	VAL	N-CA-C	-5.51	96.12	111.00
1	E	150	VAL	N-CA-C	-5.48	96.19	111.00
1	A	148	PRO	N-CA-C	-5.40	98.06	112.10
1	I	148	PRO	N-CA-C	-5.34	98.22	112.10
1	G	148	PRO	N-CA-C	-5.30	98.33	112.10
1	E	148	PRO	N-CA-C	-5.25	98.46	112.10
1	O	148	PRO	N-CA-C	-5.21	98.55	112.10
1	B	148	PRO	N-CA-C	-5.16	98.70	112.10
1	B	117	ILE	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1728	0	1766	24	0
1	B	1728	0	1766	19	0
1	C	1728	0	1766	18	0
1	D	1728	0	1766	20	0
1	E	1728	0	1766	22	0
1	F	1728	0	1766	22	0
1	G	1728	0	1766	20	0
1	H	1728	0	1766	22	0
1	I	1728	0	1766	25	0
1	J	1728	0	1766	24	0
1	K	1728	0	1766	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1728	0	1766	29	0
1	M	1728	0	1766	26	0
1	N	1728	0	1766	24	0
1	O	1728	0	1766	30	0
2	A	32	0	12	1	0
2	B	32	0	12	2	0
2	C	32	0	12	1	0
2	D	32	0	12	2	0
2	E	32	0	12	1	0
2	F	32	0	12	2	0
2	G	32	0	12	2	0
2	H	32	0	12	2	0
2	I	32	0	12	2	0
2	J	32	0	12	2	0
2	K	32	0	12	2	0
2	L	32	0	12	2	0
2	M	32	0	12	3	0
2	N	32	0	12	1	0
2	O	32	0	12	2	0
3	A	66	0	0	4	0
3	B	64	0	0	4	0
3	C	66	0	0	2	0
3	D	66	0	0	2	0
3	E	63	0	0	1	0
3	F	66	0	0	0	0
3	G	67	0	0	3	0
3	H	64	0	0	1	0
3	I	67	0	0	2	0
3	J	61	0	0	2	0
3	K	65	0	0	2	0
3	L	65	0	0	2	0
3	M	68	0	0	1	0
3	N	64	0	0	2	0
3	O	63	0	0	4	0
All	All	27375	0	26670	323	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (323) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:13:ALA:O	1:I:17:ARG:HD3	1.83	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:93:MET:HB2	1:O:95:VAL:HG23	1.72	0.71
1:C:13:ALA:O	1:C:17:ARG:HD3	1.90	0.71
1:H:93:MET:HB2	1:H:95:VAL:HG23	1.71	0.71
1:L:93:MET:HB2	1:L:95:VAL:HG23	1.73	0.71
1:F:13:ALA:O	1:F:17:ARG:HD3	1.91	0.70
1:G:13:ALA:O	1:G:17:ARG:HD3	1.91	0.70
1:M:179:HIS:HD2	3:M:580:HOH:O	1.76	0.69
1:J:93:MET:HB2	1:J:95:VAL:HG23	1.75	0.69
1:B:159:LEU:HD22	1:B:198:SER:HB3	1.75	0.68
1:H:135:SER:O	1:H:139:ARG:HG3	1.95	0.67
1:H:13:ALA:O	1:H:17:ARG:HD3	1.94	0.67
1:F:135:SER:O	1:F:139:ARG:HG3	1.95	0.67
1:A:13:ALA:O	1:A:17:ARG:HD3	1.94	0.67
1:N:13:ALA:O	1:N:17:ARG:HD3	1.94	0.66
1:K:93:MET:HB2	1:K:95:VAL:HG23	1.77	0.66
1:O:13:ALA:O	1:O:17:ARG:HD3	1.95	0.66
1:K:13:ALA:O	1:K:17:ARG:HD3	1.95	0.66
1:A:168:THR:HG22	1:A:170:ASN:H	1.61	0.66
1:M:168:THR:HG22	1:M:170:ASN:H	1.61	0.65
1:F:159:LEU:HD22	1:F:198:SER:HB3	1.78	0.65
1:K:187:ILE:HD13	1:L:139:ARG:HG2	1.78	0.65
1:G:179:HIS:HD2	3:G:467:HOH:O	1.80	0.65
1:D:93:MET:HB2	1:D:95:VAL:HG23	1.78	0.65
1:I:93:MET:HB2	1:I:95:VAL:HG23	1.79	0.65
1:C:179:HIS:HD2	3:C:578:HOH:O	1.78	0.64
1:M:159:LEU:HD22	1:M:198:SER:HB3	1.80	0.64
1:B:88:LEU:HD23	1:B:132:ILE:HA	1.79	0.64
1:D:168:THR:HG22	1:D:170:ASN:H	1.63	0.64
1:I:159:LEU:HD22	1:I:198:SER:HB3	1.80	0.64
1:C:93:MET:HB2	1:C:95:VAL:HG23	1.80	0.63
1:L:13:ALA:O	1:L:17:ARG:HD3	1.99	0.63
1:O:185:ARG:NH2	2:O:415:GTP:O2B	2.32	0.63
1:M:93:MET:HB2	1:M:95:VAL:HG23	1.80	0.63
1:M:13:ALA:O	1:M:17:ARG:HD3	2.00	0.62
1:C:135:SER:O	1:C:139:ARG:HG3	1.99	0.62
1:H:168:THR:HG22	1:H:170:ASN:H	1.64	0.62
1:B:13:ALA:O	1:B:17:ARG:HD3	1.98	0.62
1:K:168:THR:HG22	1:K:170:ASN:H	1.63	0.62
1:J:13:ALA:O	1:J:17:ARG:HD3	1.99	0.62
1:A:93:MET:HB2	1:A:95:VAL:HG23	1.81	0.62
1:L:168:THR:HG22	1:L:170:ASN:H	1.64	0.62
1:N:93:MET:HB2	1:N:95:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:13:ALA:O	1:E:17:ARG:HD3	2.00	0.61
1:G:93:MET:HB2	1:G:95:VAL:HG23	1.81	0.61
1:F:93:MET:HB2	1:F:95:VAL:HG23	1.81	0.61
1:G:168:THR:HG22	1:G:170:ASN:H	1.66	0.61
1:O:135:SER:O	1:O:139:ARG:HG3	2.01	0.61
1:D:13:ALA:O	1:D:17:ARG:HD3	2.01	0.60
1:K:11:HIS:O	1:K:15:VAL:HG23	2.01	0.60
1:B:93:MET:HB2	1:B:95:VAL:HG23	1.83	0.60
1:A:11:HIS:O	1:A:15:VAL:HG23	2.02	0.60
1:I:135:SER:O	1:I:139:ARG:HG3	2.02	0.60
1:F:168:THR:HG22	1:F:170:ASN:H	1.66	0.60
1:C:168:THR:HG22	1:C:170:ASN:H	1.68	0.59
1:I:185:ARG:HG2	1:I:186:GLY:N	2.18	0.58
1:O:168:THR:HG22	1:O:170:ASN:H	1.68	0.58
1:D:185:ARG:HG2	1:D:186:GLY:N	2.17	0.58
1:G:88:LEU:HD23	1:G:132:ILE:HA	1.86	0.58
1:I:185:ARG:NH2	2:I:409:GTP:O2B	2.37	0.58
1:E:93:MET:HB2	1:E:95:VAL:HG23	1.87	0.57
1:O:185:ARG:HG2	1:O:186:GLY:N	2.19	0.57
1:I:179:HIS:HD2	3:I:469:HOH:O	1.86	0.57
1:F:185:ARG:NH2	2:F:406:GTP:O2B	2.38	0.56
1:F:75:PHE:CE1	1:F:148:PRO:HG3	2.40	0.56
1:O:179:HIS:HD2	3:O:558:HOH:O	1.88	0.56
1:L:88:LEU:HD23	1:L:132:ILE:HA	1.88	0.56
1:A:185:ARG:HG2	1:A:186:GLY:N	2.21	0.56
1:E:132:ILE:HB	1:E:166:LEU:HD21	1.88	0.56
1:N:88:LEU:HD23	1:N:132:ILE:HA	1.88	0.56
1:H:185:ARG:HG2	1:H:186:GLY:N	2.21	0.56
1:E:159:LEU:HD22	1:E:198:SER:HB3	1.89	0.55
1:H:159:LEU:HD22	1:H:198:SER:HB3	1.88	0.55
1:J:168:THR:HG22	1:J:170:ASN:H	1.71	0.55
1:J:179:HIS:HD2	3:J:558:HOH:O	1.90	0.55
1:I:168:THR:HG22	1:I:170:ASN:H	1.73	0.54
1:O:75:PHE:CE1	1:O:148:PRO:HG3	2.43	0.54
1:K:159:LEU:HD22	1:K:198:SER:HB3	1.90	0.54
1:C:211:HIS:HB3	3:D:520:HOH:O	2.08	0.54
2:H:408:GTP:C2	1:I:134:LEU:HG	2.43	0.53
1:K:88:LEU:HD23	1:K:132:ILE:HA	1.89	0.53
1:A:16:ALA:HB3	1:A:17:ARG:HH11	1.74	0.53
1:A:88:LEU:HD23	1:A:132:ILE:HA	1.90	0.53
1:J:185:ARG:HG2	1:J:186:GLY:N	2.23	0.53
1:C:185:ARG:HG2	1:C:186:GLY:N	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:211:HIS:CD2	1:H:215:ARG:HH22	2.27	0.53
3:K:471:HOH:O	1:O:211:HIS:HB3	2.07	0.53
1:B:168:THR:HG22	1:B:170:ASN:H	1.74	0.53
1:F:11:HIS:O	1:F:15:VAL:HG23	2.08	0.53
1:I:211:HIS:HB3	3:J:520:HOH:O	2.08	0.53
1:F:88:LEU:HD23	1:F:132:ILE:HA	1.91	0.53
1:O:185:ARG:HG2	1:O:186:GLY:H	1.74	0.53
1:I:75:PHE:CE1	1:I:148:PRO:HG3	2.44	0.52
1:K:135:SER:O	1:K:139:ARG:HG3	2.09	0.52
1:D:159:LEU:HD22	1:D:198:SER:HB3	1.91	0.52
1:N:159:LEU:HD22	1:N:198:SER:HB3	1.91	0.52
1:M:211:HIS:HB3	3:N:520:HOH:O	2.10	0.52
1:N:135:SER:O	1:N:139:ARG:HG3	2.08	0.52
1:N:152:GLU:HB3	1:O:95:VAL:HG21	1.90	0.52
1:G:211:HIS:HB3	3:G:437:HOH:O	2.09	0.52
1:G:185:ARG:HG2	1:G:186:GLY:N	2.23	0.52
1:M:185:ARG:NH2	2:M:413:GTP:O2B	2.42	0.52
1:E:19:LEU:HD12	1:E:160:ILE:HG13	1.91	0.52
1:B:135:SER:O	1:B:139:ARG:HG3	2.09	0.52
1:I:142:GLN:O	1:I:146:GLN:HG2	2.10	0.52
1:L:208:ASN:O	1:L:212:GLU:HG3	2.11	0.51
1:E:138:ASN:HD22	1:E:138:ASN:H	1.56	0.51
1:F:152:GLU:HB3	1:G:95:VAL:HG21	1.92	0.51
1:M:42:HIS:O	1:M:46:ILE:HG13	2.11	0.51
1:I:16:ALA:HB3	1:I:17:ARG:HH11	1.75	0.51
3:A:463:HOH:O	1:E:211:HIS:HB3	2.10	0.51
1:N:185:ARG:HG2	1:N:186:GLY:N	2.25	0.51
1:N:211:HIS:HB3	3:O:520:HOH:O	2.09	0.51
1:A:179:HIS:HD2	3:A:455:HOH:O	1.93	0.51
1:L:11:HIS:O	1:L:15:VAL:HG23	2.11	0.51
1:C:142:GLN:O	1:C:146:GLN:HG2	2.11	0.50
1:E:179:HIS:HD2	3:E:464:HOH:O	1.93	0.50
1:A:21:THR:HG23	1:A:153:ARG:NH1	2.26	0.50
1:L:159:LEU:HD22	1:L:198:SER:HB3	1.93	0.50
1:D:185:ARG:HG2	1:D:186:GLY:H	1.75	0.50
1:G:159:LEU:HD22	1:G:198:SER:HB3	1.92	0.50
1:O:11:HIS:O	1:O:15:VAL:HG23	2.11	0.50
1:E:88:LEU:HD23	1:E:132:ILE:HA	1.94	0.50
1:K:134:LEU:HG	2:O:415:GTP:C2	2.47	0.50
1:J:159:LEU:HD22	1:J:198:SER:HB3	1.94	0.49
1:I:44:THR:HG23	1:I:54:LEU:HD13	1.93	0.49
1:G:135:SER:O	1:G:139:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:88:LEU:HD23	1:O:132:ILE:HA	1.94	0.49
1:H:211:HIS:HB3	3:I:411:HOH:O	2.11	0.49
2:G:407:GTP:C2	1:H:134:LEU:HG	2.47	0.49
1:O:179:HIS:CD2	3:O:558:HOH:O	2.65	0.49
1:D:135:SER:O	1:D:139:ARG:HG3	2.12	0.49
1:E:44:THR:HG23	1:E:54:LEU:HD13	1.93	0.49
1:O:125:TYR:CD2	1:O:166:LEU:HD13	2.48	0.49
2:F:406:GTP:C2	1:G:134:LEU:HG	2.48	0.49
2:L:412:GTP:C2	1:M:134:LEU:HG	2.48	0.49
1:M:135:SER:O	1:M:139:ARG:HG3	2.13	0.49
1:A:135:SER:O	1:A:139:ARG:HG3	2.13	0.49
1:H:88:LEU:HD23	1:H:132:ILE:HA	1.93	0.49
1:N:132:ILE:HB	1:N:166:LEU:HD21	1.94	0.49
1:O:208:ASN:O	1:O:212:GLU:HG3	2.13	0.49
1:F:95:VAL:HG21	1:J:152:GLU:HB3	1.95	0.48
1:L:212:GLU:HG2	1:L:215:ARG:NH2	2.27	0.48
1:G:11:HIS:O	1:G:15:VAL:HG23	2.13	0.48
1:K:98:MET:HA	1:K:125:TYR:O	2.13	0.48
1:L:212:GLU:HG2	1:L:215:ARG:HH21	1.78	0.48
1:G:180:TYR:CE2	1:G:183:LYS:HD3	2.48	0.48
1:I:88:LEU:HD23	1:I:132:ILE:HA	1.94	0.48
1:B:16:ALA:HB3	1:B:17:ARG:HH11	1.79	0.48
1:A:159:LEU:HD22	1:A:198:SER:HB3	1.96	0.48
1:O:168:THR:HG21	3:O:540:HOH:O	2.13	0.48
1:B:138:ASN:H	1:B:138:ASN:HD22	1.62	0.48
1:O:138:ASN:H	1:O:138:ASN:HD22	1.61	0.48
1:I:185:ARG:HG2	1:I:186:GLY:H	1.79	0.48
1:L:185:ARG:NH2	2:L:412:GTP:O2B	2.47	0.48
1:H:11:HIS:O	1:H:15:VAL:HG23	2.14	0.48
1:L:44:THR:HG23	1:L:54:LEU:HD13	1.95	0.48
1:D:11:HIS:O	1:D:15:VAL:HG23	2.14	0.48
1:M:159:LEU:O	1:M:163:GLN:HG3	2.14	0.48
1:F:211:HIS:HB3	3:G:409:HOH:O	2.13	0.48
1:L:138:ASN:H	1:L:138:ASN:HD22	1.61	0.47
1:O:16:ALA:HB3	1:O:17:ARG:HH11	1.77	0.47
1:L:185:ARG:HG2	1:L:186:GLY:N	2.30	0.47
1:L:75:PHE:CE1	1:L:148:PRO:HG3	2.49	0.47
1:J:135:SER:O	1:J:139:ARG:HG3	2.14	0.47
1:N:62:THR:HB	1:N:63:PRO:HD3	1.97	0.47
1:E:11:HIS:O	1:E:15:VAL:HG23	2.13	0.47
1:E:135:SER:O	1:E:139:ARG:HG3	2.14	0.47
1:M:90:GLU:HB3	1:M:92:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:132:ILE:HB	1:M:166:LEU:HD21	1.96	0.47
1:D:179:HIS:HD2	3:D:577:HOH:O	1.96	0.47
1:A:139:ARG:HG2	1:E:187:ILE:HD13	1.96	0.47
1:O:34:THR:O	1:O:38:LEU:HG	2.14	0.47
1:L:211:HIS:CD2	1:M:215:ARG:HH22	2.32	0.47
1:G:90:GLU:HB3	1:G:92:LYS:HE3	1.97	0.47
1:H:208:ASN:O	1:H:212:GLU:HG3	2.15	0.47
1:N:168:THR:HG22	1:N:170:ASN:H	1.80	0.47
1:B:179:HIS:HD2	3:B:558:HOH:O	1.97	0.47
1:E:183:LYS:HG3	1:E:190:ALA:HA	1.96	0.46
1:I:208:ASN:O	1:I:212:GLU:HG3	2.16	0.46
1:F:16:ALA:HB3	1:F:17:ARG:HH11	1.80	0.46
1:E:142:GLN:O	1:E:146:GLN:HG2	2.15	0.46
1:E:47:MET:CE	1:E:59:LEU:HD22	2.45	0.46
1:J:88:LEU:HD23	1:J:132:ILE:HA	1.98	0.46
1:J:56:ASP:OD2	1:J:58:SER:HB3	2.16	0.46
1:D:47:MET:CE	1:D:59:LEU:HD22	2.45	0.46
2:G:407:GTP:O1A	1:H:87:THR:HG21	2.15	0.46
1:H:142:GLN:O	1:H:146:GLN:HG2	2.16	0.46
1:N:11:HIS:O	1:N:15:VAL:HG23	2.15	0.46
1:F:208:ASN:O	1:F:212:GLU:HG3	2.16	0.46
1:C:180:TYR:CE2	1:C:183:LYS:HD3	2.51	0.46
1:L:16:ALA:HB3	1:L:17:ARG:HH11	1.81	0.46
1:F:134:LEU:HG	2:J:410:GTP:C2	2.51	0.46
1:D:208:ASN:O	1:D:212:GLU:HG3	2.15	0.46
2:C:403:GTP:C2	1:D:134:LEU:HG	2.51	0.46
1:J:142:GLN:O	1:J:146:GLN:HG2	2.15	0.46
1:M:185:ARG:HG2	1:M:186:GLY:N	2.31	0.46
2:M:413:GTP:C2	1:N:134:LEU:HG	2.51	0.46
1:F:139:ARG:HG2	1:J:187:ILE:HD13	1.98	0.46
1:O:142:GLN:O	1:O:146:GLN:HG2	2.16	0.46
1:H:19:LEU:HD12	1:H:160:ILE:HG13	1.98	0.46
1:K:8:ALA:O	1:K:12:GLU:HG3	2.16	0.46
1:D:56:ASP:OD2	1:D:58:SER:HB3	2.16	0.46
2:M:413:GTP:O3'	1:N:136:LYS:HE2	2.17	0.45
1:K:95:VAL:HG21	1:O:152:GLU:HB3	1.97	0.45
1:M:125:TYR:CD2	1:M:166:LEU:HD13	2.51	0.45
1:C:208:ASN:O	1:C:212:GLU:HG3	2.17	0.45
1:I:125:TYR:CD2	1:I:166:LEU:HD13	2.52	0.45
1:B:179:HIS:CD2	3:B:558:HOH:O	2.69	0.45
1:E:98:MET:HE1	1:E:213:PHE:HD1	1.82	0.45
1:A:34:THR:HA	1:A:37:SER:OG	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:98:MET:HA	1:H:125:TYR:O	2.16	0.45
1:N:183:LYS:HG3	1:N:190:ALA:HA	1.98	0.45
1:M:208:ASN:O	1:M:212:GLU:HG3	2.17	0.45
1:O:47:MET:CE	1:O:59:LEU:HD22	2.46	0.45
1:I:19:LEU:HD12	1:I:160:ILE:HG13	1.98	0.45
1:B:211:HIS:CD2	1:C:215:ARG:HH22	2.35	0.45
2:K:411:GTP:C2	1:L:134:LEU:HG	2.52	0.45
1:M:142:GLN:O	1:M:146:GLN:HG2	2.16	0.45
1:H:16:ALA:HB3	1:H:17:ARG:HH11	1.82	0.44
1:D:185:ARG:NH2	2:D:404:GTP:O2B	2.50	0.44
1:F:44:THR:HG23	1:F:54:LEU:HD13	1.98	0.44
2:N:414:GTP:O1A	1:O:87:THR:HG21	2.17	0.44
1:K:125:TYR:CD2	1:K:166:LEU:HD13	2.53	0.44
1:A:211:HIS:HB3	3:B:520:HOH:O	2.17	0.44
1:B:11:HIS:O	1:B:15:VAL:HG23	2.16	0.44
1:A:142:GLN:O	1:A:146:GLN:HG2	2.16	0.44
1:C:185:ARG:HG2	1:C:186:GLY:H	1.83	0.44
1:A:179:HIS:CD2	3:A:455:HOH:O	2.69	0.44
1:G:8:ALA:O	1:G:12:GLU:HG3	2.17	0.44
1:D:8:ALA:O	1:D:12:GLU:HG3	2.17	0.44
1:I:138:ASN:HD22	1:I:138:ASN:H	1.66	0.44
1:F:19:LEU:HD12	1:F:160:ILE:HG13	2.00	0.44
1:E:185:ARG:HG2	1:E:186:GLY:N	2.32	0.44
1:C:179:HIS:CD2	3:C:578:HOH:O	2.62	0.44
1:D:16:ALA:HB3	1:D:17:ARG:HH11	1.82	0.44
1:I:132:ILE:HB	1:I:166:LEU:HD21	1.99	0.44
1:M:56:ASP:OD2	1:M:58:SER:HB3	2.17	0.44
2:D:404:GTP:C2	1:E:134:LEU:HG	2.52	0.44
1:N:34:THR:O	1:N:38:LEU:HG	2.18	0.44
1:B:168:THR:HG21	3:B:540:HOH:O	2.18	0.44
1:L:187:ILE:HD13	1:M:139:ARG:HG2	1.98	0.44
1:H:44:THR:HG23	1:H:54:LEU:HD13	2.00	0.44
1:K:21:THR:HG23	1:K:153:ARG:NH1	2.32	0.44
1:O:159:LEU:HD22	1:O:198:SER:HB3	1.99	0.43
1:M:88:LEU:HD23	1:M:132:ILE:HA	2.00	0.43
1:A:208:ASN:O	1:A:212:GLU:HG3	2.18	0.43
1:A:134:LEU:HG	2:E:405:GTP:C2	2.53	0.43
1:I:47:MET:CE	1:I:59:LEU:HD22	2.48	0.43
1:K:211:HIS:CD2	1:L:215:ARG:HH22	2.37	0.43
1:M:19:LEU:HD12	1:M:160:ILE:HG13	2.00	0.43
1:K:16:ALA:HB3	1:K:17:ARG:HH11	1.83	0.43
1:C:56:ASP:OD2	1:C:58:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:8:ALA:O	1:L:12:GLU:HG3	2.19	0.43
1:I:210:ARG:O	1:I:214:LEU:HG	2.18	0.43
2:K:411:GTP:O1A	1:L:87:THR:HG21	2.19	0.43
1:G:44:THR:HG23	1:G:54:LEU:HD13	2.00	0.43
1:J:16:ALA:HB3	1:J:17:ARG:HH11	1.83	0.43
1:A:185:ARG:HG2	1:A:186:GLY:H	1.82	0.43
1:J:75:PHE:CE1	1:J:148:PRO:HG3	2.54	0.43
1:J:46:ILE:O	1:J:50:LEU:HG	2.18	0.43
1:A:168:THR:HG21	3:A:438:HOH:O	2.18	0.43
1:J:47:MET:CE	1:J:59:LEU:HD22	2.49	0.43
1:G:153:ARG:O	1:G:157:GLN:HG3	2.19	0.43
1:I:211:HIS:CD2	1:J:215:ARG:HH22	2.37	0.42
1:H:125:TYR:CD2	1:H:166:LEU:HD13	2.54	0.42
1:A:98:MET:HA	1:A:125:TYR:O	2.19	0.42
2:A:401:GTP:C2	1:B:134:LEU:HG	2.53	0.42
1:N:16:ALA:HB3	1:N:17:ARG:HH11	1.84	0.42
1:C:159:LEU:HD22	1:C:198:SER:HB3	2.01	0.42
1:F:47:MET:CE	1:F:59:LEU:HD22	2.48	0.42
1:B:185:ARG:HG2	1:B:186:GLY:N	2.34	0.42
1:F:21:THR:HG23	1:F:153:ARG:NH1	2.35	0.42
1:J:183:LYS:HG3	1:J:190:ALA:HA	2.01	0.42
1:D:34:THR:O	1:D:38:LEU:HG	2.19	0.42
1:E:16:ALA:HB3	1:E:17:ARG:HH11	1.84	0.42
1:A:44:THR:HG23	1:A:54:LEU:HD13	2.01	0.42
1:K:179:HIS:HD2	3:K:463:HOH:O	2.01	0.42
2:B:402:GTP:C2	1:C:134:LEU:HG	2.55	0.42
1:F:185:ARG:HG2	1:F:186:GLY:N	2.35	0.42
1:N:172:ALA:HB2	1:N:203:PHE:CG	2.55	0.42
1:H:168:THR:HG21	3:H:576:HOH:O	2.20	0.42
1:H:187:ILE:HD13	1:I:139:ARG:HG2	2.02	0.42
1:C:200:GLY:O	1:C:203:PHE:HB2	2.20	0.42
1:L:135:SER:O	1:L:139:ARG:HG3	2.19	0.41
1:L:13:ALA:HA	1:L:17:ARG:NH1	2.35	0.41
1:J:208:ASN:O	1:J:212:GLU:HG3	2.20	0.41
1:B:156:GLN:HG3	1:C:93:MET:HB3	2.03	0.41
1:M:62:THR:HB	1:M:63:PRO:HD3	2.02	0.41
1:O:128:LYS:HB3	1:O:129:ASP:H	1.76	0.41
1:H:185:ARG:NH2	2:H:408:GTP:O2B	2.53	0.41
1:J:185:ARG:NH2	2:J:410:GTP:O2B	2.53	0.41
1:N:192:SER:HA	1:O:102:ARG:O	2.20	0.41
1:D:187:ILE:HD13	1:E:139:ARG:HG2	2.01	0.41
1:N:115:VAL:HG12	1:N:116:THR:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:69:MET:HA	1:N:73:GLU:OE1	2.20	0.41
1:D:152:GLU:HB3	1:E:95:VAL:HG21	2.03	0.41
1:K:208:ASN:O	1:K:212:GLU:HG3	2.20	0.41
1:F:102:ARG:CZ	1:J:193:ALA:HB3	2.50	0.41
1:L:79:ASP:HB3	1:L:82:ASN:ND2	2.36	0.41
1:D:69:MET:HA	1:D:73:GLU:OE1	2.21	0.41
1:A:115:VAL:HG12	1:A:116:THR:N	2.36	0.41
1:B:185:ARG:NH2	2:B:402:GTP:O2B	2.53	0.41
1:N:179:HIS:HD2	3:N:576:HOH:O	2.02	0.41
1:L:160:ILE:HA	1:L:163:GLN:HE21	1.85	0.41
1:J:213:PHE:O	1:J:217:VAL:HG23	2.21	0.41
1:J:10:VAL:HG21	1:J:83:PHE:CZ	2.56	0.41
1:M:155:THR:HG22	1:M:198:SER:OG	2.21	0.41
1:G:19:LEU:HD12	1:G:160:ILE:HG13	2.03	0.41
1:L:182:VAL:HG22	1:M:135:SER:HB3	2.03	0.40
2:I:409:GTP:C2	1:J:134:LEU:HG	2.56	0.40
1:B:44:THR:O	1:B:48:GLN:HG3	2.21	0.40
1:G:47:MET:SD	1:G:63:PRO:HG3	2.61	0.40
1:O:8:ALA:O	1:O:12:GLU:HG3	2.20	0.40
1:L:179:HIS:HD2	3:L:578:HOH:O	2.03	0.40
1:N:185:ARG:HG2	1:N:186:GLY:H	1.85	0.40
1:K:215:ARG:HH22	1:O:211:HIS:CD2	2.39	0.40
1:L:179:HIS:CD2	3:L:578:HOH:O	2.73	0.40
1:N:142:GLN:O	1:N:146:GLN:HG2	2.21	0.40
1:M:153:ARG:O	1:M:157:GLN:HG3	2.20	0.40
1:B:44:THR:HG23	1:B:54:LEU:HD13	2.02	0.40
1:O:99:VAL:O	1:O:124:ALA:HA	2.21	0.40
1:A:183:LYS:HG3	1:A:190:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25	17
1	C	219/221 (99%)	211 (96%)	6 (3%)	2 (1%)	25	17
1	D	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	25	17
1	E	219/221 (99%)	208 (95%)	9 (4%)	2 (1%)	25	17
1	F	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	25	17
1	G	219/221 (99%)	206 (94%)	11 (5%)	2 (1%)	25	17
1	H	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25	17
1	I	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25	17
1	J	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	25	17
1	K	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25	17
1	L	219/221 (99%)	205 (94%)	12 (6%)	2 (1%)	25	17
1	M	219/221 (99%)	208 (95%)	8 (4%)	3 (1%)	16	9
1	N	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25	17
1	O	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	25	17
All	All	3285/3315 (99%)	3114 (95%)	140 (4%)	31 (1%)	25	17

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	PRO
1	I	22	PRO
1	K	22	PRO
1	L	22	PRO
1	A	22	PRO
1	A	26	PRO
1	B	26	PRO
1	C	26	PRO
1	D	26	PRO
1	E	22	PRO
1	E	26	PRO
1	F	22	PRO
1	F	26	PRO
1	G	22	PRO
1	G	26	PRO
1	H	22	PRO
1	H	26	PRO
1	I	26	PRO

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Mol	Chain	Res	Type
1	J	22	PRO
1	J	26	PRO
1	K	26	PRO
1	L	26	PRO
1	M	26	PRO
1	N	26	PRO
1	O	22	PRO
1	O	26	PRO
1	M	22	PRO
1	N	22	PRO
1	M	218	ARG
1	C	22	PRO
1	D	22	PRO

### 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%)	66	70
1	B	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	C	194/194 (100%)	191 (98%)	3 (2%)	76	81
1	D	194/194 (100%)	191 (98%)	3 (2%)	76	81
1	E	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	F	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	G	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	H	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	I	194/194 (100%)	191 (98%)	3 (2%)	76	81
1	J	194/194 (100%)	191 (98%)	3 (2%)	76	81
1	K	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	L	194/194 (100%)	191 (98%)	3 (2%)	76	81
1	M	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	N	194/194 (100%)	190 (98%)	4 (2%)	66	70
1	O	194/194 (100%)	191 (98%)	3 (2%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2910/2910 (100%)	2856 (98%)	54 (2%)	69	73

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	MET
1	A	185	ARG
1	A	219	HIS
1	A	220	HIS
1	B	93	MET
1	B	185	ARG
1	B	219	HIS
1	B	220	HIS
1	C	93	MET
1	C	219	HIS
1	C	220	HIS
1	D	93	MET
1	D	219	HIS
1	D	220	HIS
1	E	93	MET
1	E	185	ARG
1	E	219	HIS
1	E	220	HIS
1	F	93	MET
1	F	185	ARG
1	F	219	HIS
1	F	220	HIS
1	G	93	MET
1	G	185	ARG
1	G	219	HIS
1	G	220	HIS
1	H	93	MET
1	H	185	ARG
1	H	219	HIS
1	H	220	HIS
1	I	93	MET
1	I	219	HIS
1	I	220	HIS
1	J	93	MET
1	J	219	HIS
1	J	220	HIS
1	K	93	MET

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Mol	Chain	Res	Type
1	K	185	ARG
1	K	219	HIS
1	K	220	HIS
1	L	93	MET
1	L	219	HIS
1	L	220	HIS
1	M	63	PRO
1	M	93	MET
1	M	219	HIS
1	M	220	HIS
1	N	63	PRO
1	N	93	MET
1	N	219	HIS
1	N	220	HIS
1	O	93	MET
1	O	219	HIS
1	O	220	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	163	GLN
1	A	207	GLN
1	B	138	ASN
1	B	163	GLN
1	B	207	GLN
1	B	211	HIS
1	C	146	GLN
1	C	163	GLN
1	C	207	GLN
1	D	146	GLN
1	D	163	GLN
1	D	207	GLN
1	E	138	ASN
1	E	207	GLN
1	F	138	ASN
1	F	163	GLN
1	F	207	GLN
1	G	138	ASN
1	G	146	GLN
1	G	163	GLN

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Mol	Chain	Res	Type
1	G	207	GLN
1	H	138	ASN
1	H	163	GLN
1	H	207	GLN
1	I	138	ASN
1	I	163	GLN
1	I	207	GLN
1	J	138	ASN
1	J	163	GLN
1	K	42	HIS
1	K	138	ASN
1	K	146	GLN
1	K	163	GLN
1	L	138	ASN
1	L	163	GLN
1	L	207	GLN
1	M	138	ASN
1	M	163	GLN
1	M	207	GLN
1	N	42	HIS
1	N	138	ASN
1	N	163	GLN
1	N	207	GLN
1	O	138	ASN
1	O	146	GLN
1	O	163	GLN
1	O	207	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	-	34,34,34	1.47	6 (17%)	51,54,54	2.86	10 (19%)
2	GTP	B	402	-	34,34,34	1.40	7 (20%)	51,54,54	3.57	13 (25%)
2	GTP	C	403	-	34,34,34	1.77	9 (26%)	51,54,54	3.06	12 (23%)
2	GTP	D	404	-	34,34,34	1.59	8 (23%)	51,54,54	3.27	13 (25%)
2	GTP	E	405	-	34,34,34	1.48	5 (14%)	51,54,54	3.55	13 (25%)
2	GTP	F	406	-	34,34,34	1.60	4 (11%)	51,54,54	3.12	14 (27%)
2	GTP	G	407	-	34,34,34	1.73	9 (26%)	51,54,54	3.05	9 (17%)
2	GTP	H	408	-	34,34,34	1.60	10 (29%)	51,54,54	3.36	13 (25%)
2	GTP	I	409	-	34,34,34	1.65	8 (23%)	51,54,54	3.04	16 (31%)
2	GTP	J	410	-	34,34,34	1.78	9 (26%)	51,54,54	4.09	12 (23%)
2	GTP	K	411	-	34,34,34	1.57	8 (23%)	51,54,54	2.87	13 (25%)
2	GTP	L	412	-	34,34,34	1.48	8 (23%)	51,54,54	3.46	14 (27%)
2	GTP	M	413	-	34,34,34	1.66	8 (23%)	51,54,54	2.81	16 (31%)
2	GTP	N	414	-	34,34,34	1.69	6 (17%)	51,54,54	3.66	11 (21%)
2	GTP	O	415	-	34,34,34	1.71	6 (17%)	51,54,54	3.68	16 (31%)

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	-	-	0/22/38/38	0/1/3/3
2	GTP	B	402	-	-	0/22/38/38	0/1/3/3
2	GTP	C	403	-	-	0/22/38/38	0/1/3/3
2	GTP	D	404	-	-	0/22/38/38	0/1/3/3
2	GTP	E	405	-	-	0/22/38/38	0/1/3/3
2	GTP	F	406	-	-	0/22/38/38	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	G	407	-	-	0/22/38/38	0/1/3/3
2	GTP	H	408	-	-	0/22/38/38	0/1/3/3
2	GTP	I	409	-	-	0/22/38/38	0/1/3/3
2	GTP	J	410	-	-	0/22/38/38	0/1/3/3
2	GTP	K	411	-	-	0/22/38/38	0/1/3/3
2	GTP	L	412	-	-	0/22/38/38	0/1/3/3
2	GTP	M	413	-	-	0/22/38/38	0/1/3/3
2	GTP	N	414	-	-	0/22/38/38	0/1/3/3
2	GTP	O	415	-	-	0/22/38/38	0/1/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	410	GTP	PG-O3B	5.06	1.69	1.60
2	N	414	GTP	PG-O3B	4.65	1.68	1.60
2	F	406	GTP	PA-O3A	4.36	1.67	1.59
2	N	414	GTP	PA-O3A	4.26	1.67	1.59
2	C	403	GTP	PG-O3B	4.23	1.67	1.60
2	J	410	GTP	PA-O3A	4.15	1.67	1.59
2	K	411	GTP	PA-O3A	4.08	1.67	1.59
2	O	415	GTP	PA-O3A	4.05	1.67	1.59
2	I	409	GTP	PG-O3B	3.95	1.67	1.60
2	G	407	GTP	PG-O3B	3.88	1.66	1.60
2	G	407	GTP	PA-O3A	3.86	1.66	1.59
2	E	405	GTP	PA-O3A	3.80	1.66	1.59
2	H	408	GTP	PA-O3A	3.63	1.66	1.59
2	M	413	GTP	PG-O3B	3.62	1.66	1.60
2	B	402	GTP	PA-O3A	3.57	1.66	1.59
2	I	409	GTP	PA-O3A	3.55	1.66	1.59
2	O	415	GTP	PG-O3B	3.47	1.66	1.60
2	C	403	GTP	PA-O3A	3.45	1.66	1.59
2	H	408	GTP	C2'-C1'	-3.40	1.48	1.53
2	D	404	GTP	PG-O3B	3.33	1.66	1.60
2	K	411	GTP	O6-C6	-3.21	1.18	1.24
2	K	411	GTP	C2'-C1'	-3.21	1.48	1.53
2	A	401	GTP	PA-O3A	3.17	1.65	1.59
2	N	414	GTP	C2'-C1'	-3.11	1.49	1.53
2	K	411	GTP	PG-O3B	3.08	1.65	1.60
2	M	413	GTP	C2'-C1'	-3.07	1.49	1.53
2	E	405	GTP	O6-C6	-3.00	1.18	1.24
2	A	401	GTP	C2'-C1'	-2.99	1.49	1.53
2	F	406	GTP	O6-C6	-2.97	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	415	GTP	C2-N1	2.96	1.41	1.36
2	M	413	GTP	C6-C5	2.94	1.46	1.41
2	C	403	GTP	C2'-C1'	-2.92	1.49	1.53
2	F	406	GTP	PG-O3B	2.92	1.65	1.60
2	J	410	GTP	C2-N1	2.91	1.41	1.36
2	L	412	GTP	O4'-C4'	2.91	1.51	1.45
2	I	409	GTP	O6-C6	-2.86	1.18	1.24
2	N	414	GTP	O4'-C4'	2.78	1.51	1.45
2	E	405	GTP	O4'-C4'	2.77	1.51	1.45
2	A	401	GTP	O6-C6	-2.76	1.19	1.24
2	M	413	GTP	PA-O3A	2.75	1.64	1.59
2	D	404	GTP	C2-N1	2.70	1.41	1.36
2	D	404	GTP	C2'-C1'	-2.69	1.49	1.53
2	A	401	GTP	PG-O3B	2.69	1.64	1.60
2	I	409	GTP	PB-O2B	-2.69	1.43	1.55
2	B	402	GTP	O4'-C4'	2.69	1.51	1.45
2	M	413	GTP	O6-C6	-2.69	1.19	1.24
2	D	404	GTP	C6-N1	2.69	1.41	1.37
2	G	407	GTP	O6-C6	-2.68	1.19	1.24
2	E	405	GTP	PG-O3B	2.65	1.64	1.60
2	F	406	GTP	O4'-C4'	2.62	1.51	1.45
2	M	413	GTP	C2-N1	2.62	1.40	1.36
2	O	415	GTP	C2-N2	2.59	1.36	1.32
2	D	404	GTP	C6-C5	2.56	1.45	1.41
2	L	412	GTP	C2'-C1'	-2.52	1.49	1.53
2	L	412	GTP	PG-O3B	2.49	1.64	1.60
2	O	415	GTP	O4'-C4'	2.48	1.50	1.45
2	O	415	GTP	O6-C6	-2.48	1.19	1.24
2	B	402	GTP	O6-C6	-2.45	1.19	1.24
2	G	407	GTP	C6-C5	2.43	1.45	1.41
2	H	408	GTP	PG-O3B	2.42	1.64	1.60
2	I	409	GTP	O4'-C4'	2.42	1.50	1.45
2	D	404	GTP	PA-O3A	2.42	1.64	1.59
2	I	409	GTP	C2'-C1'	-2.40	1.50	1.53
2	C	403	GTP	C2-N1	2.38	1.40	1.36
2	J	410	GTP	PB-O3B	2.37	1.64	1.59
2	H	408	GTP	O4'-C4'	2.37	1.50	1.45
2	J	410	GTP	O6-C6	-2.37	1.19	1.24
2	G	407	GTP	C2'-C1'	-2.35	1.50	1.53
2	C	403	GTP	O6-C6	-2.34	1.19	1.24
2	J	410	GTP	C2-N2	2.33	1.36	1.32
2	N	414	GTP	O6-C6	-2.33	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	412	GTP	C2-N1	2.31	1.40	1.36
2	H	408	GTP	PB-O2B	-2.31	1.44	1.55
2	M	413	GTP	C4-N9	-2.28	1.34	1.37
2	L	412	GTP	PB-O2B	-2.26	1.45	1.55
2	L	412	GTP	C2-N2	2.26	1.35	1.32
2	C	403	GTP	PB-O2B	-2.24	1.45	1.55
2	I	409	GTP	C2-N1	2.24	1.40	1.36
2	D	404	GTP	O2'-C2'	2.22	1.48	1.43
2	H	408	GTP	C4-N9	-2.20	1.34	1.37
2	J	410	GTP	O4'-C4'	2.20	1.50	1.45
2	G	407	GTP	O4'-C4'	2.20	1.50	1.45
2	G	407	GTP	PB-O3B	2.18	1.63	1.59
2	A	401	GTP	PB-O2B	-2.17	1.45	1.55
2	G	407	GTP	C2-N1	2.17	1.40	1.36
2	G	407	GTP	O2'-C2'	2.17	1.48	1.43
2	H	408	GTP	O2'-C2'	2.16	1.48	1.43
2	C	403	GTP	C6-C5	2.16	1.44	1.41
2	B	402	GTP	PB-O2B	-2.16	1.45	1.55
2	B	402	GTP	PA-O2A	-2.15	1.45	1.55
2	B	402	GTP	C4-N9	-2.14	1.34	1.37
2	E	405	GTP	PB-O2B	-2.13	1.45	1.55
2	A	401	GTP	PB-O3A	-2.12	1.56	1.59
2	D	404	GTP	C4-N3	2.12	1.39	1.35
2	L	412	GTP	PA-O3A	2.12	1.63	1.59
2	C	403	GTP	O2'-C2'	2.11	1.48	1.43
2	I	409	GTP	O4'-C1'	2.11	1.44	1.41
2	B	402	GTP	C2'-C1'	-2.11	1.50	1.53
2	H	408	GTP	PB-O1B	-2.11	1.43	1.51
2	K	411	GTP	C5-C4	-2.09	1.35	1.40
2	K	411	GTP	O4'-C4'	2.08	1.49	1.45
2	C	403	GTP	C2-N2	2.07	1.35	1.32
2	L	412	GTP	O6-C6	-2.07	1.20	1.24
2	J	410	GTP	C5-C4	-2.07	1.35	1.40
2	J	410	GTP	C6-N1	2.05	1.40	1.37
2	K	411	GTP	C2-N2	2.03	1.35	1.32
2	M	413	GTP	O4'-C4'	2.03	1.49	1.45
2	N	414	GTP	C5-C4	-2.02	1.35	1.40
2	H	408	GTP	C2-N2	2.01	1.35	1.32
2	H	408	GTP	C6-C5	2.00	1.44	1.41
2	K	411	GTP	PB-O3B	2.00	1.63	1.59

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	410	GTP	C6-C5-N7	-26.70	130.54	134.14
2	O	415	GTP	C6-C5-N7	-23.26	131.01	134.14
2	N	414	GTP	C6-C5-N7	-23.17	131.02	134.14
2	B	402	GTP	C6-C5-N7	-22.24	131.15	134.14
2	E	405	GTP	C6-C5-N7	-22.09	131.16	134.14
2	L	412	GTP	C6-C5-N7	-21.05	131.31	134.14
2	H	408	GTP	C6-C5-N7	-20.51	131.38	134.14
2	D	404	GTP	C6-C5-N7	-20.00	131.45	134.14
2	F	406	GTP	C6-C5-N7	-18.61	131.63	134.14
2	C	403	GTP	C6-C5-N7	-18.24	131.68	134.14
2	G	407	GTP	C6-C5-N7	-17.96	131.72	134.14
2	I	409	GTP	C6-C5-N7	-17.68	131.76	134.14
2	A	401	GTP	C6-C5-N7	-16.57	131.91	134.14
2	K	411	GTP	C6-C5-N7	-16.36	131.94	134.14
2	M	413	GTP	C6-C5-N7	-15.58	132.04	134.14
2	H	408	GTP	C4'-O4'-C1'	-6.20	103.02	109.75
2	L	412	GTP	C4'-O4'-C1'	-6.17	103.05	109.75
2	B	402	GTP	C4'-O4'-C1'	-6.10	103.12	109.75
2	K	411	GTP	C4'-O4'-C1'	-5.90	103.33	109.75
2	A	401	GTP	C4'-O4'-C1'	-5.75	103.50	109.75
2	E	405	GTP	C4'-O4'-C1'	-5.73	103.52	109.75
2	G	407	GTP	C4'-O4'-C1'	-5.70	103.56	109.75
2	F	406	GTP	C4'-O4'-C1'	-5.55	103.72	109.75
2	M	413	GTP	C4'-O4'-C1'	-5.55	103.72	109.75
2	N	414	GTP	C4'-O4'-C1'	-5.50	103.78	109.75
2	J	410	GTP	C4'-O4'-C1'	-5.47	103.81	109.75
2	C	403	GTP	C4'-O4'-C1'	-5.43	103.85	109.75
2	D	404	GTP	C4'-O4'-C1'	-5.30	104.00	109.75
2	I	409	GTP	C4'-O4'-C1'	-5.23	104.07	109.75
2	O	415	GTP	C4'-O4'-C1'	-5.07	104.24	109.75
2	B	402	GTP	C8-N9-C4	-4.28	103.64	106.90
2	A	401	GTP	C8-N9-C4	-3.68	104.09	106.90
2	H	408	GTP	O4'-C4'-C5'	3.60	122.22	109.36
2	G	407	GTP	C8-N9-C1'	3.60	133.48	126.38
2	N	414	GTP	O4'-C4'-C5'	3.58	122.13	109.36
2	E	405	GTP	O4'-C4'-C5'	3.55	122.02	109.36
2	K	411	GTP	C8-N9-C4	-3.54	104.19	106.90
2	K	411	GTP	C8-N9-C1'	3.53	133.34	126.38
2	J	410	GTP	C8-N9-C1'	3.48	133.24	126.38
2	M	413	GTP	C8-N9-C1'	3.47	133.22	126.38
2	D	404	GTP	O4'-C4'-C5'	3.47	121.75	109.36
2	N	414	GTP	C8-N9-C4	-3.44	104.27	106.90
2	L	412	GTP	O4'-C4'-C5'	3.42	121.56	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	410	GTP	O4'-C4'-C5'	3.40	121.50	109.36
2	G	407	GTP	O4'-C4'-C5'	3.39	121.48	109.36
2	M	413	GTP	O4'-C4'-C5'	3.39	121.48	109.36
2	B	402	GTP	C8-N9-C1'	3.37	133.03	126.38
2	D	404	GTP	C8-N9-C1'	3.37	133.02	126.38
2	N	414	GTP	C8-N9-C1'	3.35	132.99	126.38
2	A	401	GTP	C8-N9-C1'	3.35	132.98	126.38
2	L	412	GTP	C8-N9-C1'	3.34	132.95	126.38
2	F	406	GTP	O4'-C4'-C5'	3.33	121.25	109.36
2	A	401	GTP	O4'-C4'-C5'	3.29	121.10	109.36
2	B	402	GTP	O4'-C4'-C5'	3.28	121.07	109.36
2	I	409	GTP	O4'-C4'-C5'	3.27	121.05	109.36
2	I	409	GTP	C8-N9-C1'	3.23	132.74	126.38
2	F	406	GTP	C8-N9-C1'	3.23	132.74	126.38
2	C	403	GTP	O4'-C4'-C5'	3.20	120.80	109.36
2	E	405	GTP	C8-N9-C4	-3.19	104.47	106.90
2	C	403	GTP	C8-N9-C1'	3.17	132.62	126.38
2	G	407	GTP	C8-N9-C4	-3.13	104.51	106.90
2	K	411	GTP	O4'-C4'-C5'	3.12	120.51	109.36
2	E	405	GTP	C8-N9-C1'	3.12	132.53	126.38
2	O	415	GTP	C8-N9-C1'	3.11	132.52	126.38
2	O	415	GTP	O4'-C4'-C5'	3.06	120.27	109.36
2	H	408	GTP	C6-N1-C2	3.05	124.84	119.51
2	K	411	GTP	C6-N1-C2	3.02	124.79	119.51
2	E	405	GTP	C6-N1-C2	3.02	124.79	119.51
2	O	415	GTP	C3'-C2'-C1'	-2.99	96.23	100.91
2	H	408	GTP	C8-N9-C1'	2.98	132.25	126.38
2	L	412	GTP	C3'-C2'-C1'	-2.98	96.25	100.91
2	M	413	GTP	C8-N9-C4	-2.95	104.64	106.90
2	L	412	GTP	C8-N9-C4	-2.94	104.66	106.90
2	L	412	GTP	C6-N1-C2	2.92	124.61	119.51
2	H	408	GTP	C8-N9-C4	-2.90	104.68	106.90
2	F	406	GTP	PB-O3B-PG	-2.90	123.17	131.68
2	O	415	GTP	C8-N9-C4	-2.90	104.69	106.90
2	C	403	GTP	C6-N1-C2	2.90	124.58	119.51
2	H	408	GTP	C3'-C2'-C1'	-2.88	96.39	100.91
2	I	409	GTP	C6-N1-C2	2.87	124.53	119.51
2	D	404	GTP	C8-N9-C4	-2.85	104.72	106.90
2	N	414	GTP	C6-N1-C2	2.84	124.47	119.51
2	D	404	GTP	C3'-C2'-C1'	-2.82	96.50	100.91
2	I	409	GTP	C8-N9-C4	-2.78	104.78	106.90
2	D	404	GTP	C6-N1-C2	2.78	124.37	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	405	GTP	O2G-PG-O1G	2.76	119.48	110.44
2	I	409	GTP	C3'-C2'-C1'	-2.76	96.58	100.91
2	C	403	GTP	C8-N9-C4	-2.76	104.79	106.90
2	B	402	GTP	O4'-C1'-N9	2.76	111.00	108.44
2	C	403	GTP	C3'-C2'-C1'	-2.76	96.59	100.91
2	J	410	GTP	C8-N9-C4	-2.74	104.81	106.90
2	A	401	GTP	C6-N1-C2	2.72	124.27	119.51
2	I	409	GTP	O2G-PG-O1G	2.72	119.33	110.44
2	B	402	GTP	C6-N1-C2	2.72	124.26	119.51
2	J	410	GTP	C1'-N9-C4	-2.71	121.95	126.64
2	C	403	GTP	O5'-PA-O1A	-2.71	98.76	109.37
2	M	413	GTP	C6-N1-C2	2.71	124.24	119.51
2	K	411	GTP	C3'-C2'-C1'	-2.71	96.67	100.91
2	L	412	GTP	O2G-PG-O1G	2.69	119.25	110.44
2	G	407	GTP	C1'-N9-C4	-2.68	122.01	126.64
2	E	405	GTP	C5'-C4'-C3'	-2.67	104.51	115.21
2	O	415	GTP	C6-N1-C2	2.65	124.15	119.51
2	F	406	GTP	C6-N1-C2	2.65	124.14	119.51
2	M	413	GTP	C1'-N9-C4	-2.61	122.13	126.64
2	H	408	GTP	C5'-C4'-C3'	-2.60	104.78	115.21
2	M	413	GTP	C3'-C2'-C1'	-2.58	96.86	100.91
2	J	410	GTP	O2G-PG-O1G	2.57	118.84	110.44
2	I	409	GTP	PB-O3B-PG	-2.56	124.18	131.68
2	O	415	GTP	O2G-PG-O1G	2.54	118.75	110.44
2	D	404	GTP	C1'-N9-C4	-2.54	122.25	126.64
2	L	412	GTP	O2A-PA-O3A	2.52	117.10	105.14
2	G	407	GTP	C6-N1-C2	2.52	123.92	119.51
2	F	406	GTP	C8-N9-C4	-2.52	104.98	106.90
2	F	406	GTP	C1'-N9-C4	-2.52	122.29	126.64
2	M	413	GTP	O5'-PA-O1A	-2.51	99.54	109.37
2	C	403	GTP	C5'-C4'-C3'	-2.49	105.24	115.21
2	N	414	GTP	C5'-C4'-C3'	-2.48	105.27	115.21
2	I	409	GTP	O5'-PA-O1A	-2.48	99.66	109.37
2	E	405	GTP	O5'-PA-O1A	-2.47	99.69	109.37
2	L	412	GTP	C1'-N9-C4	-2.46	122.39	126.64
2	O	415	GTP	C5'-C4'-C3'	-2.46	105.37	115.21
2	N	414	GTP	C3'-C2'-C1'	-2.45	97.07	100.91
2	I	409	GTP	C5'-C4'-C3'	-2.43	105.46	115.21
2	B	402	GTP	O2G-PG-O1G	2.42	118.36	110.44
2	H	408	GTP	O2A-PA-O3A	2.42	116.61	105.14
2	K	411	GTP	C1'-N9-C4	-2.41	122.46	126.64
2	M	413	GTP	C5'-C4'-C3'	-2.41	105.56	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	412	GTP	C5'-C4'-C3'	-2.40	105.58	115.21
2	I	409	GTP	C1'-N9-C4	-2.40	122.48	126.64
2	J	410	GTP	C5'-C4'-C3'	-2.39	105.63	115.21
2	J	410	GTP	C6-N1-C2	2.38	123.67	119.51
2	D	404	GTP	O2G-PG-O1G	2.37	118.20	110.44
2	L	412	GTP	PB-O3B-PG	-2.37	124.73	131.68
2	D	404	GTP	C5'-C4'-C3'	-2.35	105.81	115.21
2	C	403	GTP	C1'-N9-C4	-2.35	122.58	126.64
2	E	405	GTP	PB-O3B-PG	-2.34	124.82	131.68
2	I	409	GTP	O2B-PB-O3B	2.34	116.23	105.14
2	B	402	GTP	C5'-C4'-C3'	-2.33	105.86	115.21
2	M	413	GTP	O2G-PG-O1G	2.33	118.06	110.44
2	H	408	GTP	O2G-PG-O1G	2.33	118.05	110.44
2	F	406	GTP	O2G-PG-O1G	2.32	118.02	110.44
2	F	406	GTP	C3'-C2'-C1'	-2.31	97.29	100.91
2	G	407	GTP	C5'-C4'-C3'	-2.31	105.96	115.21
2	F	406	GTP	C5'-C4'-C3'	-2.31	105.97	115.21
2	A	401	GTP	C5'-C4'-C3'	-2.30	105.99	115.21
2	B	402	GTP	O2A-PA-O3A	2.30	116.04	105.14
2	D	404	GTP	PB-O3B-PG	-2.29	124.96	131.68
2	J	410	GTP	C3'-C2'-C1'	-2.29	97.33	100.91
2	I	409	GTP	O2A-PA-O3A	2.28	115.97	105.14
2	J	410	GTP	O5'-C5'-C4'	-2.28	100.58	108.94
2	O	415	GTP	O3A-PB-O3B	2.27	106.28	101.66
2	N	414	GTP	C1'-N9-C4	-2.26	122.73	126.64
2	O	415	GTP	PB-O3B-PG	-2.25	125.07	131.68
2	C	403	GTP	O2G-PG-O1G	2.24	117.78	110.44
2	F	406	GTP	O2B-PB-O3B	2.24	115.75	105.14
2	O	415	GTP	C1'-N9-C4	-2.22	122.80	126.64
2	L	412	GTP	O2'-C2'-C3'	2.22	119.05	111.83
2	H	408	GTP	PB-O3B-PG	-2.22	125.18	131.68
2	C	403	GTP	O2B-PB-O3B	2.21	115.63	105.14
2	M	413	GTP	PB-O3B-PG	-2.21	125.20	131.68
2	G	407	GTP	C3'-C2'-C1'	-2.20	97.46	100.91
2	K	411	GTP	C5'-C4'-C3'	-2.19	106.44	115.21
2	M	413	GTP	O2B-PB-O3B	2.19	115.51	105.14
2	D	404	GTP	O2A-PA-O3A	2.18	115.48	105.14
2	L	412	GTP	PA-O3A-PB	-2.16	125.34	131.68
2	M	413	GTP	O2A-PA-O1A	2.16	124.28	112.21
2	B	402	GTP	C3'-C2'-C1'	-2.15	97.54	100.91
2	A	401	GTP	C1'-N9-C4	-2.15	122.92	126.64
2	O	415	GTP	O2'-C2'-C3'	2.14	118.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	409	GTP	O2'-C2'-C3'	2.14	118.80	111.83
2	E	405	GTP	O2B-PB-O3B	2.12	115.21	105.14
2	F	406	GTP	O5'-C5'-C4'	-2.12	101.14	108.94
2	K	411	GTP	O3'-C3'-C2'	2.12	118.72	111.83
2	N	414	GTP	O2G-PG-O1G	2.11	117.33	110.44
2	E	405	GTP	C1'-N9-C4	-2.11	123.00	126.64
2	O	415	GTP	O5'-C5'-C4'	-2.10	101.22	108.94
2	O	415	GTP	O2A-PA-O3A	2.10	115.10	105.14
2	E	405	GTP	O5'-C5'-C4'	-2.09	101.28	108.94
2	B	402	GTP	O4'-C1'-C2'	2.09	109.97	106.77
2	N	414	GTP	O2A-PA-O3A	2.08	115.01	105.14
2	H	408	GTP	C1'-N9-C4	-2.07	123.05	126.64
2	J	410	GTP	O2B-PB-O3B	2.07	114.96	105.14
2	A	401	GTP	O2A-PA-O3A	2.07	114.95	105.14
2	A	401	GTP	O5'-C5'-C4'	-2.05	101.43	108.94
2	I	409	GTP	O5'-C5'-C4'	-2.05	101.43	108.94
2	H	408	GTP	O2'-C2'-C3'	2.04	118.49	111.83
2	K	411	GTP	O2'-C2'-C3'	2.04	118.48	111.83
2	F	406	GTP	O5'-PA-O1A	-2.04	101.39	109.37
2	K	411	GTP	PB-O3B-PG	-2.03	125.73	131.68
2	M	413	GTP	O2'-C2'-C3'	2.03	118.44	111.83
2	B	402	GTP	PB-O3B-PG	-2.03	125.74	131.68
2	K	411	GTP	O2A-PA-O3A	2.02	114.71	105.14
2	D	404	GTP	O2'-C2'-C3'	2.02	118.40	111.83
2	O	415	GTP	O2B-PB-O3B	2.02	114.70	105.14
2	M	413	GTP	O5'-C5'-C4'	-2.00	101.58	108.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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