



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 01:31 pm GMT

PDB ID : 1WPL  
Title : Crystal structure of the inhibitory form of rat GTP cyclohydrolase I/GFRP complex  
Authors : Maita, N.; Hatakeyama, K.; Okada, K.; Hakoshima, T.  
Deposited on : 2004-09-08  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

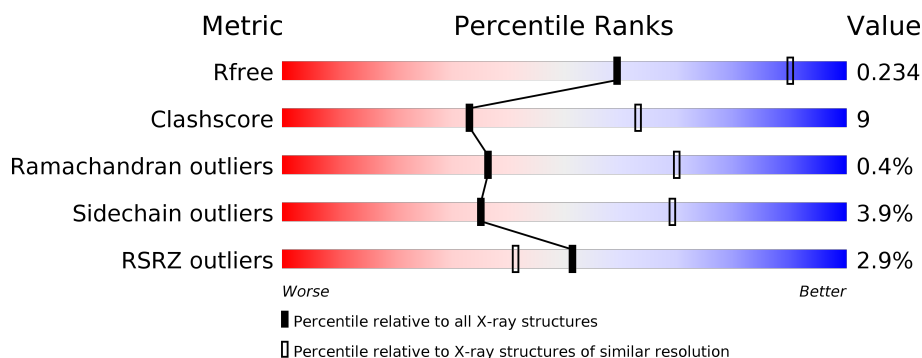
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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






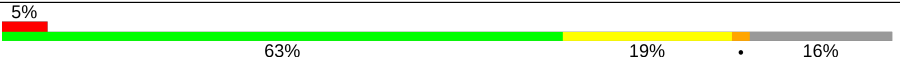
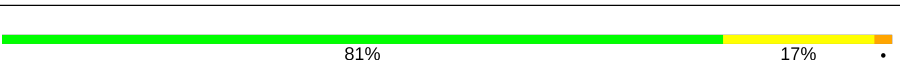

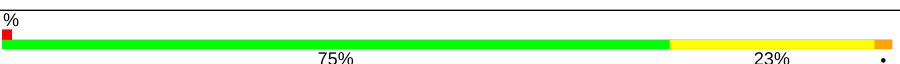
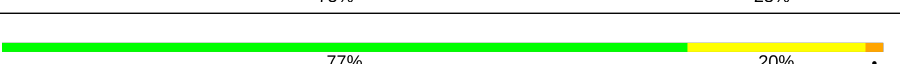
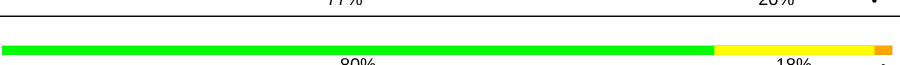
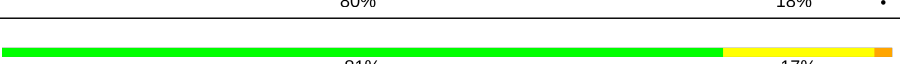
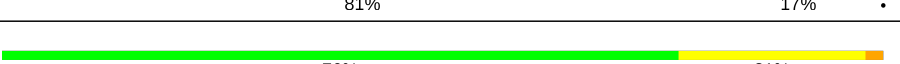
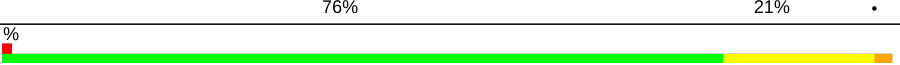

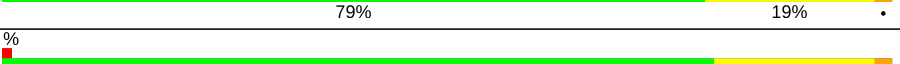
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	230	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	230	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	230	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	230	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>18%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	230	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>18%</div> <div>•</div> <div>16%</div> </div> </div>
1	F	230	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	230	
1	H	230	
1	I	230	
1	J	230	
2	K	84	
2	L	84	
2	M	84	
2	N	84	
2	O	84	
2	P	84	
2	Q	84	
2	R	84	
2	S	84	
2	T	84	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	3PO	B	2001	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22650 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GTP cyclohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	B	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	C	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	D	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	E	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	F	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	G	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	H	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	I	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			
1	J	194	Total	C	N	O	S	0	0	0
			1534	966	269	288	11			

- Molecule 2 is a protein called GTP cyclohydrolase I feedback regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	L	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	M	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	N	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			

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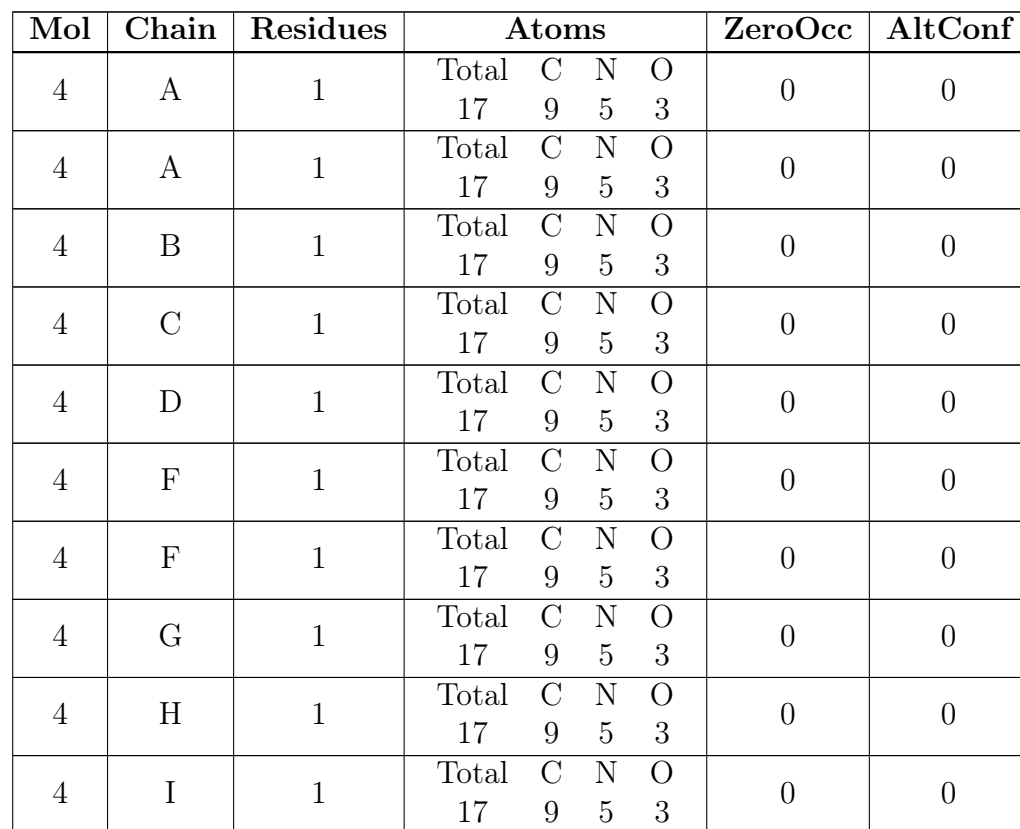
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	P	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	Q	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	R	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	S	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	T	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			

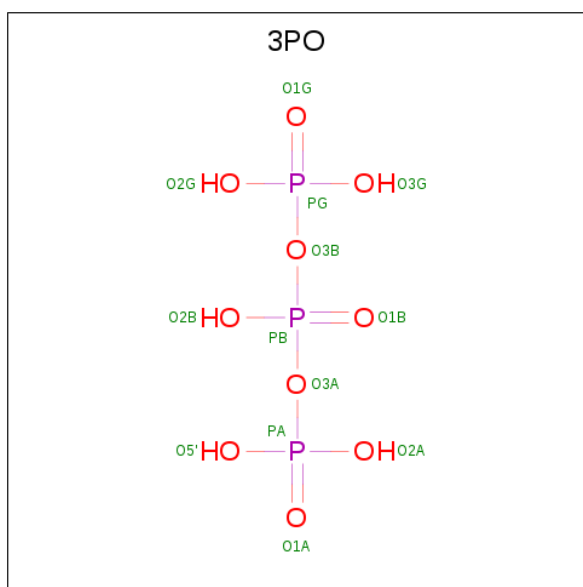
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 7,8-DIHYDROBIOPTERIN (three-letter code: HBI) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



- Molecule 5 is TRIPHOSPHATE (three-letter code: 3PO) (formula:  $\text{H}_5\text{O}_{10}\text{P}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			13	10	3		
5	B	1	Total	O	P	0	0
			13	10	3		
5	C	1	Total	O	P	0	0
			13	10	3		
5	D	1	Total	O	P	0	0
			13	10	3		
5	E	1	Total	O	P	0	0
			13	10	3		
5	F	1	Total	O	P	0	0
			13	10	3		
5	G	1	Total	O	P	0	0
			13	10	3		
5	H	1	Total	O	P	0	0
			13	10	3		
5	I	1	Total	O	P	0	0
			13	10	3		
5	J	1	Total	O	P	0	0
			13	10	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Na	0	0
			1	1		
6	Q	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total 1	Na 1	0	0
6	T	1	Total 1	Na 1	0	0
6	N	1	Total 1	Na 1	0	0
6	O	1	Total 1	Na 1	0	0
6	R	1	Total 1	Na 1	0	0
6	L	1	Total 1	Na 1	0	0
6	S	1	Total 1	Na 1	0	0
6	M	1	Total 1	Na 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total 16	O 16	0	0
7	B	13	Total 13	O 13	0	0
7	C	13	Total 13	O 13	0	0
7	D	18	Total 18	O 18	0	0
7	E	9	Total 9	O 9	0	0
7	F	15	Total 15	O 15	0	0
7	G	12	Total 12	O 12	0	0
7	H	9	Total 9	O 9	0	0
7	I	12	Total 12	O 12	0	0
7	J	12	Total 12	O 12	0	0
7	K	11	Total 11	O 11	0	0

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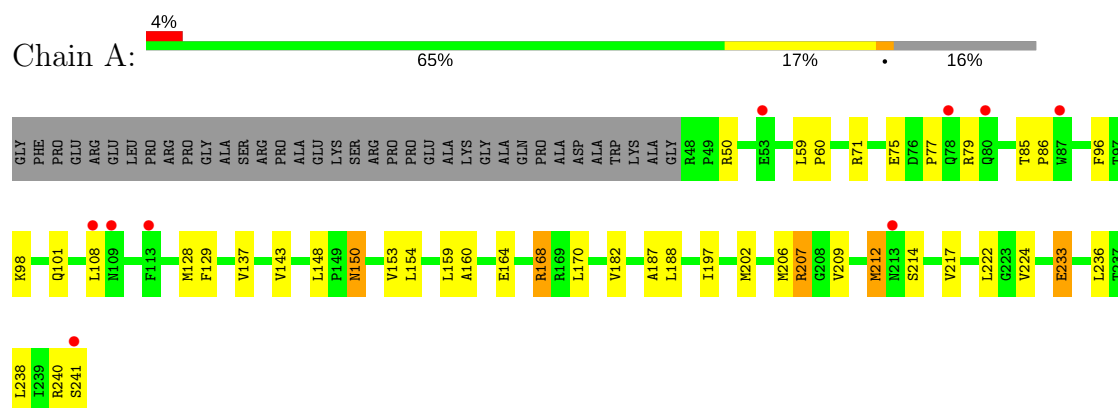
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	10	Total	O	0	0
			10	10		
7	M	8	Total	O	0	0
			8	8		
7	N	9	Total	O	0	0
			9	9		
7	O	12	Total	O	0	0
			12	12		
7	P	8	Total	O	0	0
			8	8		
7	Q	13	Total	O	0	0
			13	13		
7	R	8	Total	O	0	0
			8	8		
7	S	13	Total	O	0	0
			13	13		
7	T	9	Total	O	0	0
			9	9		

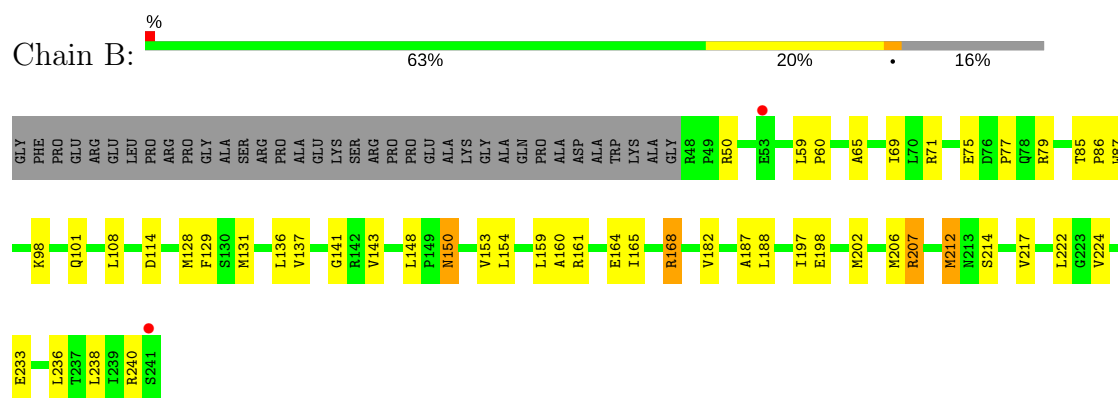
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

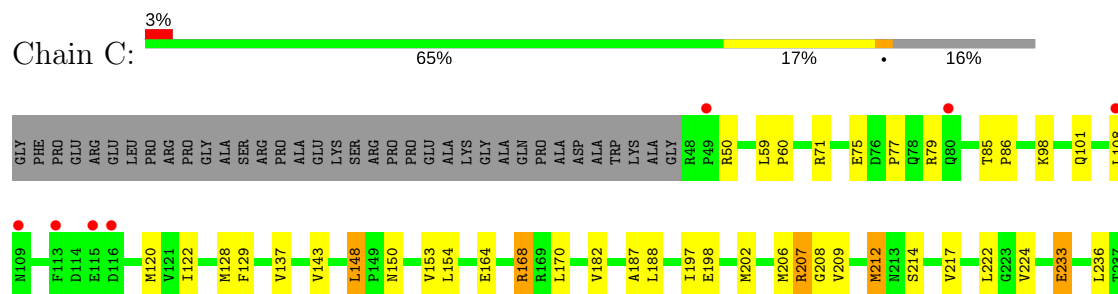
#### • Molecule 1: GTP cyclohydrolase I



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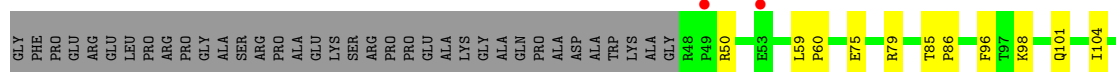


#### • Molecule 1: GTP cyclohydrolase I

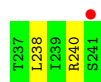
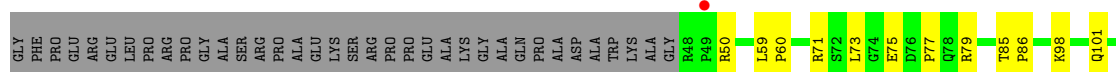




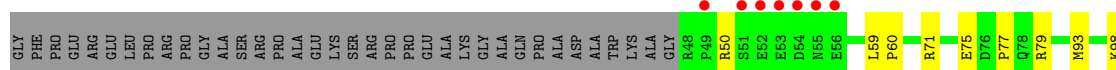
## ● Molecule 1: GTP cyclohydrolase I



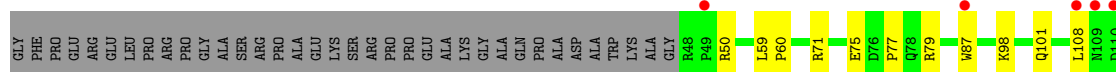
## ● Molecule 1: GTP cyclohydrolase I



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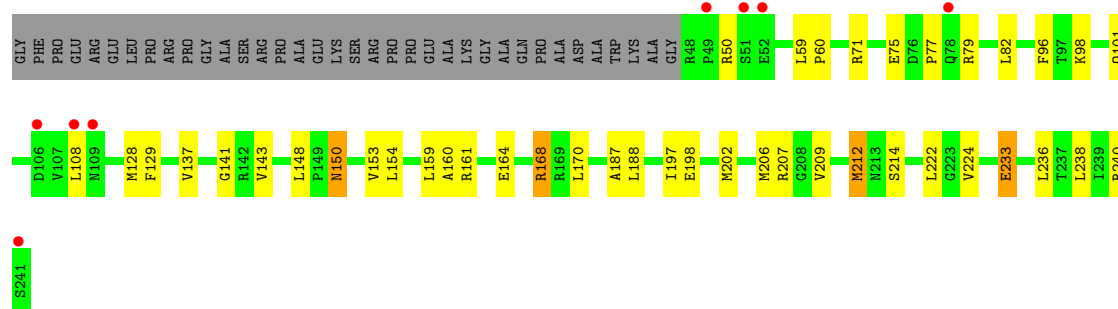


## ● Molecule 1: GTP cyclohydrolase I

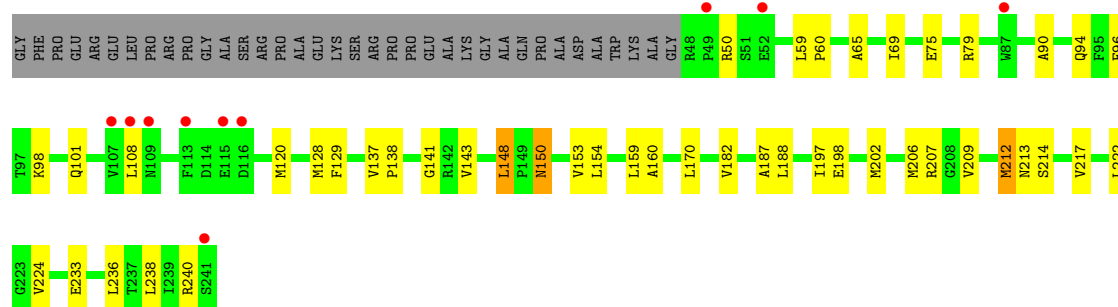




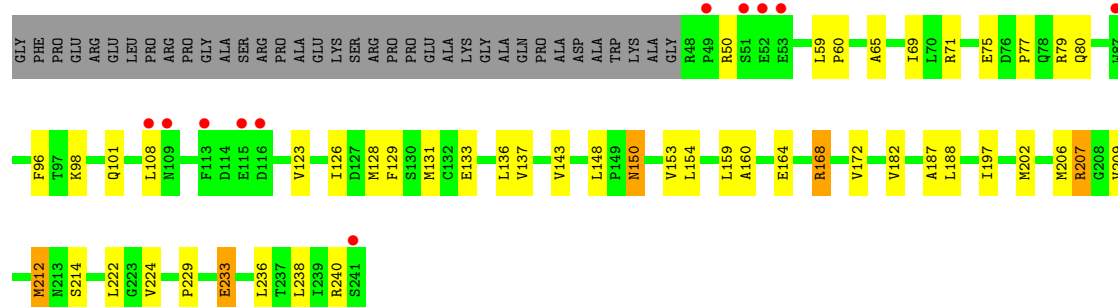
• Molecule 1: GTP cyclohydrolase I




• Molecule 1: GTP cyclohydrolase I



• Molecule 1: GTP cyclohydrolase I




• Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain K:  81% 17%




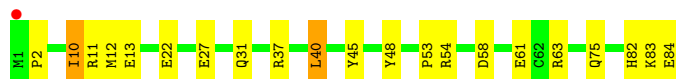
- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain L:  83% 14%




- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain M:  75% 23%



- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain N:  77% 20%




- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain O:  80% 18%




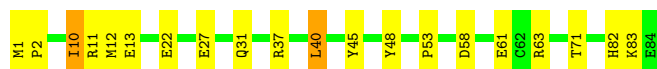
- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain P:  81% 17%




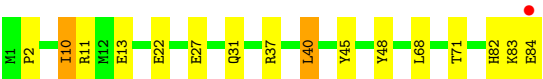
- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

Chain Q:  76% 21%

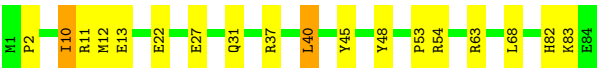
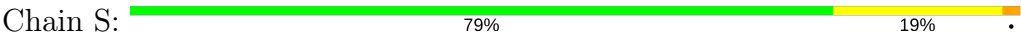


- Molecule 2: GTP cyclohydrolase I feedback regulatory protein

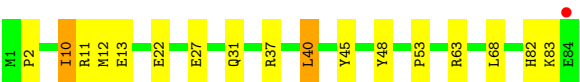
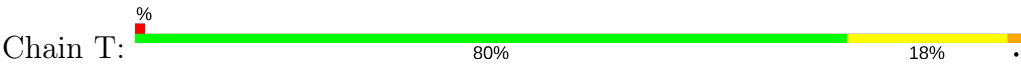
Chain R:  81% 17%



● Molecule 2: GTP cyclohydrolase I feedback regulatory protein



● Molecule 2: GTP cyclohydrolase I feedback regulatory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.72Å 109.67Å 130.27Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 29.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.80) 100.0 (29.90-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.233 0.205 , 0.234	Depositor DCC
$R_{free}$ test set	4228 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3587e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, HBI, 3PO

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	0.44	0/1559	0.66	0/2105
1	B	0.42	0/1559	0.67	0/2105
1	C	0.44	0/1559	0.67	0/2105
1	D	0.44	0/1559	0.67	0/2105
1	E	0.44	0/1559	0.67	0/2105
1	F	0.42	0/1559	0.67	0/2105
1	G	0.44	0/1559	0.66	0/2105
1	H	0.43	0/1559	0.66	0/2105
1	I	0.44	0/1559	0.66	0/2105
1	J	0.43	0/1559	0.67	1/2105 (0.0%)
2	K	0.43	0/690	0.66	0/931
2	L	0.42	0/690	0.65	0/931
2	M	0.43	0/690	0.65	0/931
2	N	0.42	0/690	0.65	0/931
2	O	0.42	0/690	0.65	0/931
2	P	0.42	0/690	0.66	0/931
2	Q	0.41	0/690	0.66	0/931
2	R	0.41	0/690	0.65	0/931
2	S	0.42	0/690	0.66	0/931
2	T	0.43	0/690	0.66	0/931
All	All	0.43	0/22490	0.66	1/30360 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	172	VAL	N-CA-C	-5.00	97.50	111.00

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	1534	0	1550	41	0
1	B	1534	0	1550	41	0
1	C	1534	0	1550	40	0
1	D	1534	0	1550	41	0
1	E	1534	0	1550	37	0
1	F	1534	0	1550	40	0
1	G	1534	0	1550	43	0
1	H	1534	0	1550	39	0
1	I	1534	0	1550	37	0
1	J	1534	0	1550	43	0
2	K	676	0	678	13	0
2	L	676	0	678	11	0
2	M	676	0	678	16	0
2	N	676	0	677	14	0
2	O	676	0	678	12	0
2	P	676	0	678	14	0
2	Q	676	0	678	16	0
2	R	676	0	678	13	0
2	S	676	0	678	12	0
2	T	676	0	678	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	34	0	26	0	0
4	B	17	0	13	0	0
4	C	17	0	13	0	0
4	D	17	0	13	0	0
4	F	34	0	26	0	0
4	G	17	0	13	0	0
4	H	17	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	17	0	13	0	0
5	A	13	0	0	0	0
5	B	13	0	0	0	0
5	C	13	0	0	0	0
5	D	13	0	0	0	0
5	E	13	0	0	0	0
5	F	13	0	0	0	0
5	G	13	0	0	0	0
5	H	13	0	0	0	0
5	I	13	0	0	0	0
5	J	13	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
7	A	16	0	0	2	0
7	B	13	0	0	1	0
7	C	13	0	0	1	0
7	D	18	0	0	1	0
7	E	9	0	0	0	0
7	F	15	0	0	1	0
7	G	12	0	0	1	0
7	H	9	0	0	1	0
7	I	12	0	0	0	0
7	J	12	0	0	1	0
7	K	11	0	0	0	0
7	L	10	0	0	0	0
7	M	8	0	0	3	0
7	N	9	0	0	0	0
7	O	12	0	0	0	0
7	P	8	0	0	2	0
7	Q	13	0	0	1	0
7	R	8	0	0	0	0
7	S	13	0	0	1	0
7	T	9	0	0	0	0
All	All	22650	0	22409	417	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 417 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:C:240:ARG:NH2	1:D:240:ARG:HH21	1.73	0.84
1:G:240:ARG:NH2	1:H:240:ARG:HH21	1.79	0.81
1:F:240:ARG:HH21	1:J:240:ARG:NH2	1.80	0.79
1:C:240:ARG:HH22	1:D:240:ARG:HH21	1.29	0.79
1:I:224:VAL:HG12	2:S:10:ILE:HD13	1.63	0.79

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	192/230 (84%)	183 (95%)	9 (5%)	0	100	100
1	B	192/230 (84%)	185 (96%)	7 (4%)	0	100	100
1	C	192/230 (84%)	183 (95%)	9 (5%)	0	100	100
1	D	192/230 (84%)	185 (96%)	7 (4%)	0	100	100
1	E	192/230 (84%)	184 (96%)	8 (4%)	0	100	100
1	F	192/230 (84%)	185 (96%)	7 (4%)	0	100	100
1	G	192/230 (84%)	183 (95%)	9 (5%)	0	100	100
1	H	192/230 (84%)	185 (96%)	7 (4%)	0	100	100
1	I	192/230 (84%)	184 (96%)	8 (4%)	0	100	100
1	J	192/230 (84%)	184 (96%)	8 (4%)	0	100	100
2	K	82/84 (98%)	77 (94%)	4 (5%)	1 (1%)	14	42
2	L	82/84 (98%)	77 (94%)	4 (5%)	1 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	82/84 (98%)	77 (94%)	4 (5%)	1 (1%)	14	42
2	N	82/84 (98%)	77 (94%)	4 (5%)	1 (1%)	14	42
2	O	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	14	42
2	P	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	14	42
2	Q	82/84 (98%)	77 (94%)	4 (5%)	1 (1%)	14	42
2	R	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	14	42
2	S	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	14	42
2	T	82/84 (98%)	77 (94%)	4 (5%)	1 (1%)	14	42
All	All	2740/3140 (87%)	2609 (95%)	121 (4%)	10 (0%)	36	70

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	10	ILE
2	L	10	ILE
2	M	10	ILE
2	R	10	ILE
2	N	10	ILE

### 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	170/196 (87%)	161 (95%)	9 (5%)	25	57
1	B	170/196 (87%)	162 (95%)	8 (5%)	29	62
1	C	170/196 (87%)	161 (95%)	9 (5%)	25	57
1	D	170/196 (87%)	161 (95%)	9 (5%)	25	57
1	E	170/196 (87%)	161 (95%)	9 (5%)	25	57
1	F	170/196 (87%)	163 (96%)	7 (4%)	33	67
1	G	170/196 (87%)	162 (95%)	8 (5%)	29	62
1	H	170/196 (87%)	160 (94%)	10 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	170/196 (87%)	163 (96%)	7 (4%)	33	67
1	J	170/196 (87%)	161 (95%)	9 (5%)	25	57
2	K	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	L	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	M	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	N	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	O	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	P	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	Q	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	R	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	S	76/76 (100%)	75 (99%)	1 (1%)	71	92
2	T	76/76 (100%)	75 (99%)	1 (1%)	71	92
All	All	2460/2720 (90%)	2365 (96%)	95 (4%)	35	69

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	236	LEU
1	G	150	ASN
2	M	40	LEU
1	F	128	MET
1	F	212	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	43	ASN
2	M	75	GLN
2	S	75	GLN
2	M	9	GLN
2	M	82	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 20 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	HBI	A	1003	-	14,18,18	2.56	6 (42%)	11,26,26	1.14	0
4	HBI	A	1004	-	14,18,18	2.45	6 (42%)	11,26,26	1.08	0
5	3PO	A	2005	-	10,12,12	1.31	1 (10%)	11,20,20	1.12	1 (9%)
4	HBI	B	1005	-	14,18,18	2.51	6 (42%)	11,26,26	1.13	0
5	3PO	B	2001	-	10,12,12	1.68	2 (20%)	11,20,20	1.13	1 (9%)
4	HBI	C	1001	-	14,18,18	2.40	4 (28%)	11,26,26	1.26	0
5	3PO	C	2002	-	10,12,12	1.47	1 (10%)	11,20,20	1.15	2 (18%)
4	HBI	D	1002	-	14,18,18	2.51	6 (42%)	11,26,26	1.17	0
5	3PO	D	2003	-	10,12,12	1.65	1 (10%)	11,20,20	1.11	1 (9%)
5	3PO	E	2004	-	10,12,12	1.51	1 (10%)	11,20,20	1.10	1 (9%)
4	HBI	F	1009	-	14,18,18	2.51	7 (50%)	11,26,26	1.13	0
4	HBI	F	1010	-	14,18,18	2.54	7 (50%)	11,26,26	1.12	0
5	3PO	F	2010	-	10,12,12	1.54	2 (20%)	11,20,20	1.17	2 (18%)
4	HBI	G	1006	-	14,18,18	2.54	7 (50%)	11,26,26	1.06	0
5	3PO	G	2006	-	10,12,12	1.15	0	11,20,20	1.16	1 (9%)
4	HBI	H	1007	-	14,18,18	2.52	7 (50%)	11,26,26	1.19	0
5	3PO	H	2007	-	10,12,12	1.57	2 (20%)	11,20,20	1.13	2 (18%)
4	HBI	I	1008	-	14,18,18	2.60	6 (42%)	11,26,26	1.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	3PO	I	2008	-	10,12,12	1.63	2 (20%)	11,20,20	1.17	2 (18%)
5	3PO	J	2009	-	10,12,12	1.34	2 (20%)	11,20,20	1.21	2 (18%)

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
4	HBI	A	1003	-	-	0/4/17/17	0/2/2/2
4	HBI	A	1004	-	-	0/4/17/17	0/2/2/2
5	3PO	A	2005	-	-	0/12/12/12	0/0/0/0
4	HBI	B	1005	-	-	0/4/17/17	0/2/2/2
5	3PO	B	2001	-	-	0/12/12/12	0/0/0/0
4	HBI	C	1001	-	-	0/4/17/17	0/2/2/2
5	3PO	C	2002	-	-	0/12/12/12	0/0/0/0
4	HBI	D	1002	-	-	0/4/17/17	0/2/2/2
5	3PO	D	2003	-	-	0/12/12/12	0/0/0/0
5	3PO	E	2004	-	-	0/12/12/12	0/0/0/0
4	HBI	F	1009	-	-	0/4/17/17	0/2/2/2
4	HBI	F	1010	-	-	0/4/17/17	0/2/2/2
5	3PO	F	2010	-	-	0/12/12/12	0/0/0/0
4	HBI	G	1006	-	-	0/4/17/17	0/2/2/2
5	3PO	G	2006	-	-	0/12/12/12	0/0/0/0
4	HBI	H	1007	-	-	0/4/17/17	0/2/2/2
5	3PO	H	2007	-	-	0/12/12/12	0/0/0/0
4	HBI	I	1008	-	-	0/4/17/17	0/2/2/2
5	3PO	I	2008	-	-	0/12/12/12	0/0/0/0
5	3PO	J	2009	-	-	0/12/12/12	0/0/0/0

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1010	HBI	O9-C9	2.06	1.46	1.42
4	D	1002	HBI	C4A-C8A	2.07	1.47	1.41
5	B	2001	3PO	PA-O3A	2.08	1.63	1.60
4	A	1004	HBI	C4A-C8A	2.09	1.47	1.41
4	F	1009	HBI	C4A-N5	2.14	1.42	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	D	2003	3PO	O2A-PA-O1A	2.03	118.53	110.60
5	H	2007	3PO	PB-O3A-PA	2.08	139.63	132.63
5	I	2008	3PO	PB-O3A-PA	2.09	139.67	132.63
5	I	2008	3PO	O2A-PA-O1A	2.12	118.85	110.60
5	C	2002	3PO	PB-O3A-PA	2.12	139.76	132.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	194/230 (84%)	-0.24	9 (4%) 32 22	11, 30, 58, 69	0
1	B	194/230 (84%)	-0.33	2 (1%) 82 77	13, 30, 57, 65	0
1	C	194/230 (84%)	-0.24	8 (4%) 37 27	12, 29, 58, 68	0
1	D	194/230 (84%)	-0.34	4 (2%) 63 54	11, 28, 56, 66	0
1	E	194/230 (84%)	-0.17	7 (3%) 42 32	11, 29, 58, 68	0
1	F	194/230 (84%)	-0.25	10 (5%) 27 18	13, 29, 58, 66	0
1	G	194/230 (84%)	-0.22	9 (4%) 32 22	13, 28, 58, 69	0
1	H	194/230 (84%)	-0.28	8 (4%) 37 27	12, 29, 56, 67	0
1	I	194/230 (84%)	-0.20	10 (5%) 27 18	13, 30, 58, 68	0
1	J	194/230 (84%)	-0.20	11 (5%) 24 15	14, 31, 58, 69	0
2	K	84/84 (100%)	-0.36	0 100 100	23, 32, 49, 58	0
2	L	84/84 (100%)	-0.41	1 (1%) 79 72	22, 31, 49, 58	0
2	M	84/84 (100%)	-0.30	1 (1%) 79 72	22, 31, 49, 59	0
2	N	84/84 (100%)	-0.41	0 100 100	22, 31, 48, 57	0
2	O	84/84 (100%)	-0.42	0 100 100	22, 32, 50, 58	0
2	P	84/84 (100%)	-0.35	0 100 100	23, 33, 50, 59	0
2	Q	84/84 (100%)	-0.29	0 100 100	25, 34, 51, 58	0
2	R	84/84 (100%)	-0.43	1 (1%) 79 72	23, 33, 49, 59	0
2	S	84/84 (100%)	-0.46	0 100 100	23, 33, 50, 58	0
2	T	84/84 (100%)	-0.33	1 (1%) 79 72	23, 33, 49, 59	0
All	All	2780/3140 (88%)	-0.29	82 (2%) 51 41	11, 31, 54, 69	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	LEU	6.7
1	G	109	ASN	5.2
1	E	241	SER	4.8
1	I	108	LEU	4.7
1	G	108	LEU	4.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	3PO	I	2008	13/13	0.73	0.35	93,96,98,99	0
5	3PO	D	2003	13/13	0.73	0.30	89,92,94,95	0
5	3PO	B	2001	13/13	0.73	0.46	98,101,102,104	0
5	3PO	J	2009	13/13	0.77	0.34	89,94,96,96	0
5	3PO	E	2004	13/13	0.77	0.28	82,91,97,98	0
5	3PO	C	2002	13/13	0.77	0.38	89,91,95,96	0
6	NA	N	1013	1/1	0.79	0.32	52,52,52,52	0
5	3PO	H	2007	13/13	0.80	0.34	89,94,96,96	0
5	3PO	F	2010	13/13	0.81	0.34	93,96,98,98	0
6	NA	K	1015	1/1	0.82	0.27	43,43,43,43	0
5	3PO	A	2005	13/13	0.83	0.31	82,83,85,86	0
6	NA	T	1016	1/1	0.83	0.23	44,44,44,44	0
6	NA	P	1017	1/1	0.86	0.20	33,33,33,33	0
6	NA	R	1019	1/1	0.88	0.29	40,40,40,40	0
5	3PO	G	2006	13/13	0.89	0.27	78,84,86,87	0
6	NA	S	1020	1/1	0.89	0.23	39,39,39,39	0
6	NA	O	1014	1/1	0.90	0.36	41,41,41,41	0
6	NA	Q	1018	1/1	0.92	0.32	51,51,51,51	0
3	ZN	C	1103	1/1	0.92	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	L	1011	1/1	0.93	0.47	35,35,35,35	0
6	NA	M	1012	1/1	0.93	0.18	35,35,35,35	0
3	ZN	G	1101	1/1	0.94	0.09	57,57,57,57	0
4	HBI	A	1003	17/17	0.95	0.14	22,26,34,35	0
3	ZN	B	1108	1/1	0.95	0.09	59,59,59,59	0
3	ZN	D	1104	1/1	0.95	0.06	58,58,58,58	0
4	HBI	D	1002	17/17	0.96	0.15	18,22,29,30	0
3	ZN	H	1107	1/1	0.96	0.08	59,59,59,59	0
4	HBI	F	1010	17/17	0.96	0.15	24,28,32,33	0
3	ZN	J	1106	1/1	0.96	0.07	56,56,56,56	0
4	HBI	B	1005	17/17	0.96	0.17	24,29,39,42	0
4	HBI	A	1004	17/17	0.96	0.15	20,23,33,34	0
4	HBI	C	1001	17/17	0.96	0.15	17,23,31,33	0
3	ZN	A	1110	1/1	0.96	0.04	60,60,60,60	0
4	HBI	F	1009	17/17	0.96	0.13	21,28,31,32	0
4	HBI	G	1006	17/17	0.97	0.14	17,19,26,30	0
4	HBI	I	1008	17/17	0.97	0.14	28,31,37,39	0
3	ZN	I	1109	1/1	0.97	0.08	51,51,51,51	0
3	ZN	E	1102	1/1	0.97	0.05	46,46,46,46	0
4	HBI	H	1007	17/17	0.97	0.14	20,25,37,40	0
3	ZN	F	1105	1/1	0.99	0.04	50,50,50,50	0

## 6.5 Other polymers

There are no such residues in this entry.