



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 10:20 AM BST

PDB ID : 1IS8
Title : Crystal structure of rat GTPCHI/GFRP stimulatory complex plus Zn
Authors : Maita, N.; Okada, K.; Hatakeyama, K.; Hakoshima, T.
Deposited on : 2001-11-18
Resolution : 2.70 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

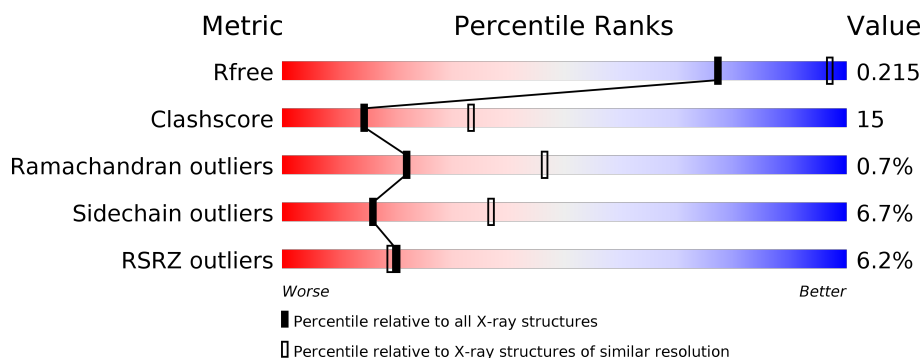
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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>11%</div> <div> <div>54%</div> <div>26%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	230	<div> <div>6%</div> <div> <div>58%</div> <div>22%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	230	<div> <div>7%</div> <div> <div>57%</div> <div>24%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	230	<div> <div>7%</div> <div> <div>56%</div> <div>26%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	230	<div> <div>5%</div> <div> <div>57%</div> <div>23%</div> <div>•</div> <div>17%</div> </div> </div>
1	F	230	<div> <div>5%</div> <div> <div>53%</div> <div>29%</div> <div>•</div> <div>17%</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	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22511 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	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	B	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	C	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	D	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	E	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	F	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	G	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	H	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	I	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	11			
1	J	192	Total	C	N	O	S	0	0	0
			1524	959	269	285	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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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 POTASSIUM ION (three-letter code: K) (formula: K).

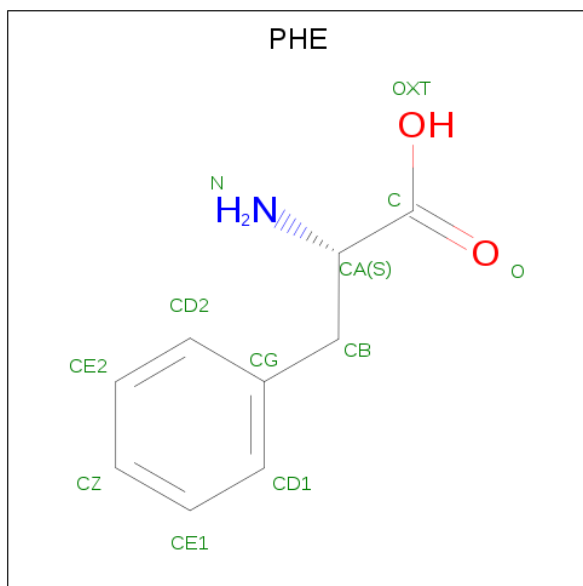
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	K	0	0
			1	1		

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

- Molecule 5 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C N O 12 9 1 2	0	0
5	M	1	Total C N O 12 9 1 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			12	9	1	2		
5	N	1	Total	C	N	O	0	0
			12	9	1	2		
5	O	1	Total	C	N	O	0	0
			12	9	1	2		
5	P	1	Total	C	N	O	0	0
			12	9	1	2		
5	Q	1	Total	C	N	O	0	0
			12	9	1	2		
5	R	1	Total	C	N	O	0	0
			12	9	1	2		
5	S	1	Total	C	N	O	0	0
			12	9	1	2		
5	T	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	18	Total	O	0	0
			18	18		
6	C	13	Total	O	0	0
			13	13		
6	D	10	Total	O	0	0
			10	10		
6	E	13	Total	O	0	0
			13	13		
6	F	15	Total	O	0	0
			15	15		
6	G	16	Total	O	0	0
			16	16		
6	H	21	Total	O	0	0
			21	21		
6	I	20	Total	O	0	0
			20	20		
6	J	20	Total	O	0	0
			20	20		
6	K	17	Total	O	0	0
			17	17		

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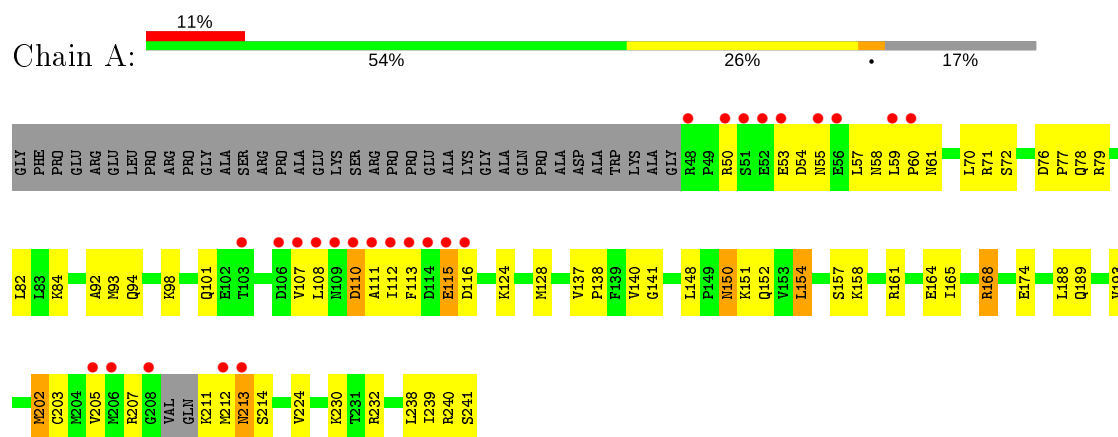
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	19	Total	O	0	0
			19	19		
6	M	16	Total	O	0	0
			16	16		
6	N	16	Total	O	0	0
			16	16		
6	O	16	Total	O	0	0
			16	16		
6	P	27	Total	O	0	0
			27	27		
6	Q	31	Total	O	0	0
			31	31		
6	R	28	Total	O	0	0
			28	28		
6	S	22	Total	O	0	0
			22	22		
6	T	16	Total	O	0	0
			16	16		

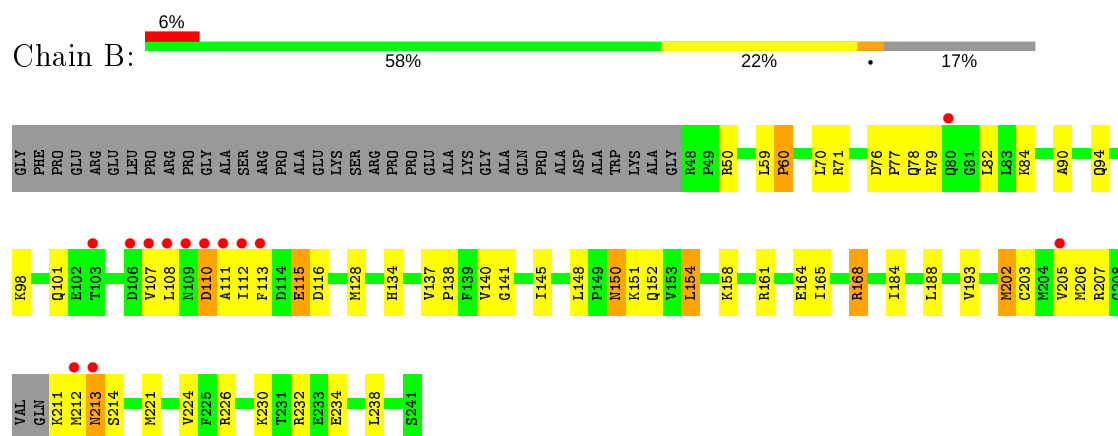
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

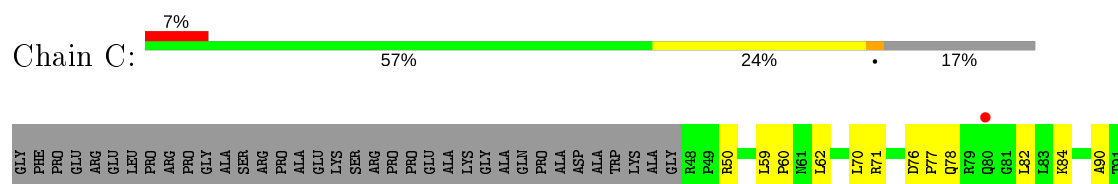
• Molecule 1: GTP Cyclohydrolase I

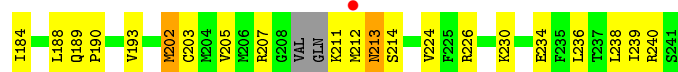


• Molecule 1: GTP Cyclohydrolase I

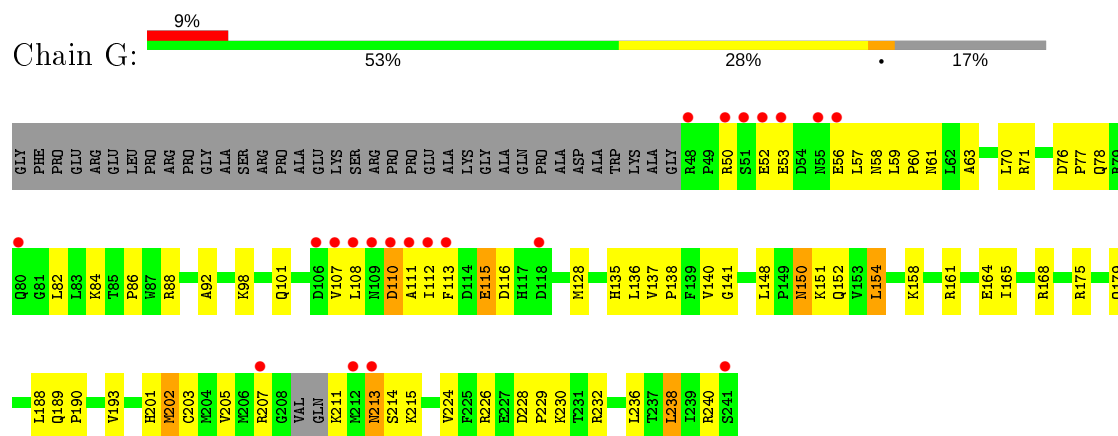


• Molecule 1: GTP Cyclohydrolase I

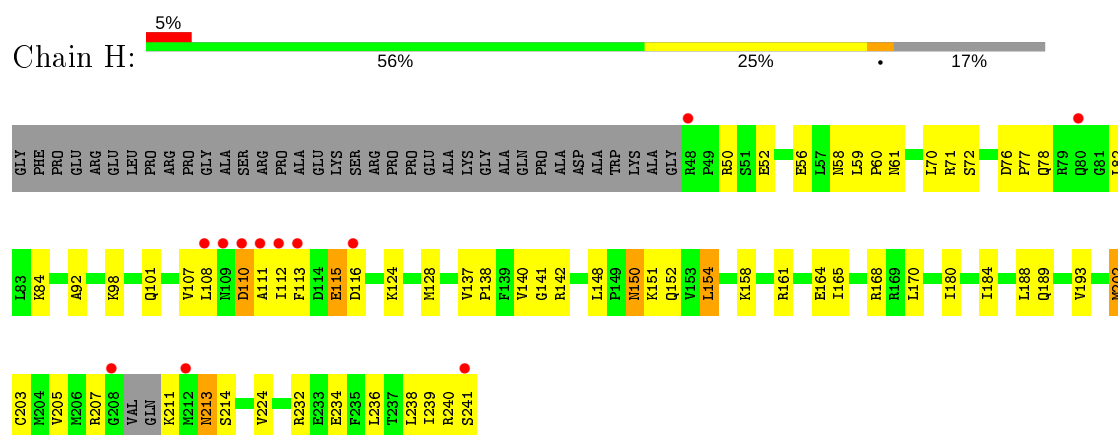




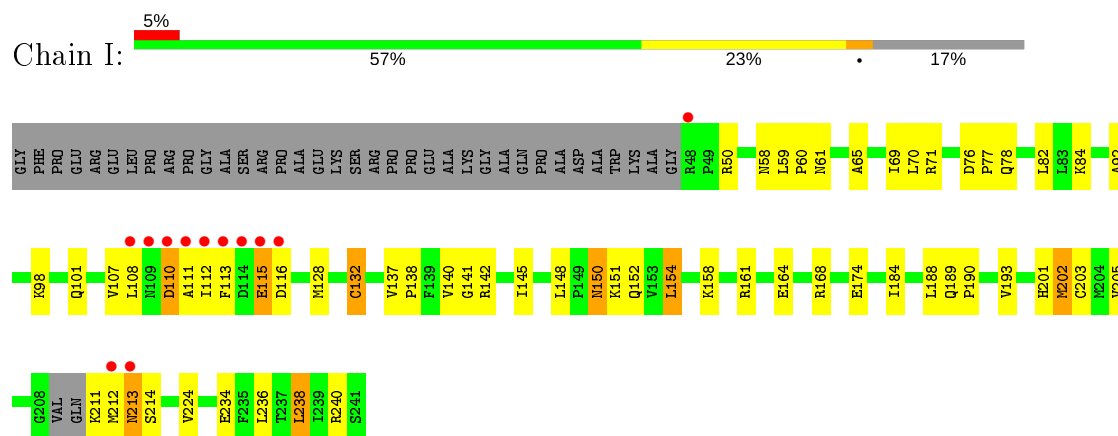
- Molecule 1: GTP Cyclohydrolase I



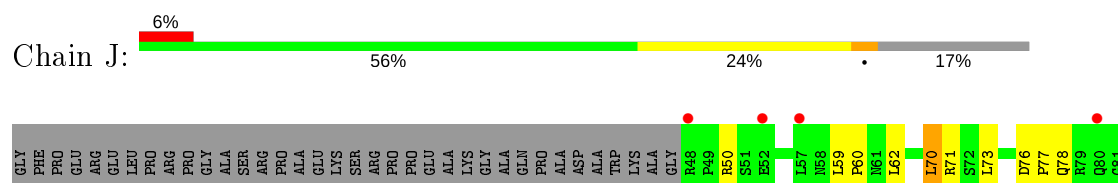
- Molecule 1: GTP Cyclohydrolase I

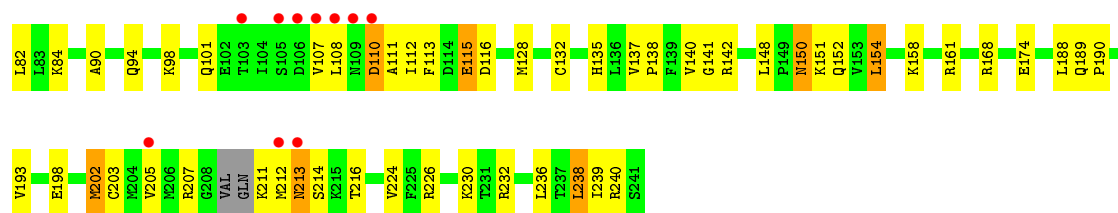


- Molecule 1: GTP Cyclohydrolase I

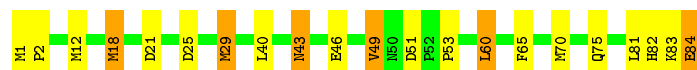
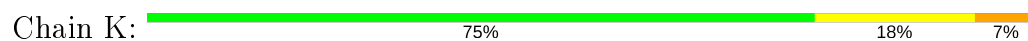


- Molecule 1: GTP Cyclohydrolase I

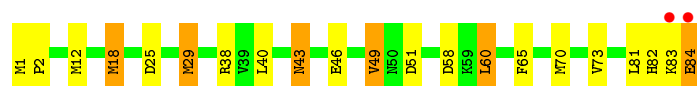
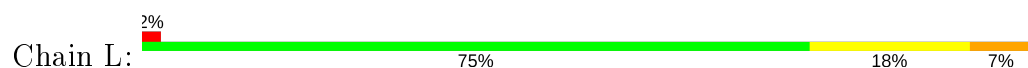




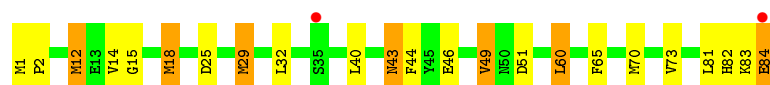
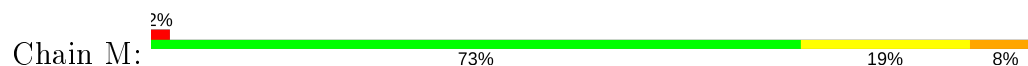
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



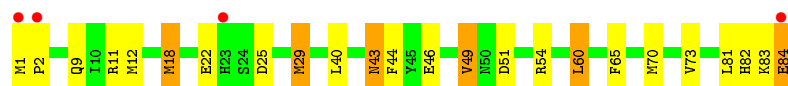
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



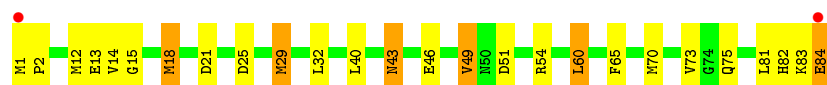
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



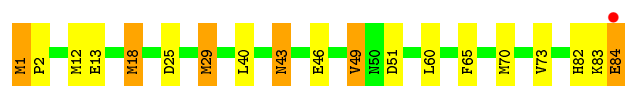
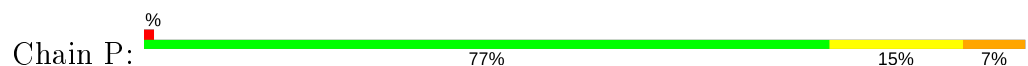
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein




● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

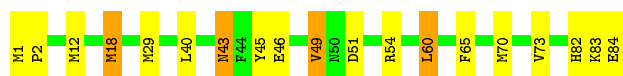


● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



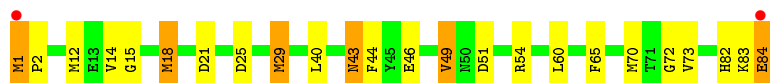
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain Q:  77% 18% 5%



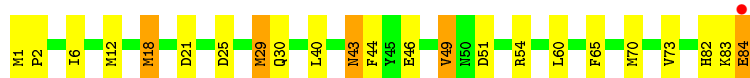
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain R:  2% 71% 21% 7%




- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain S:  % 73% 21% 6%



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain T:  4% 75% 20% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.90Å 111.43Å 125.91Å 90.00° 97.32° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 29.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.70) 95.5 (29.65-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.68Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.219 , 0.245 0.215 , 0.215	Depositor DCC
R_{free} test set	4648 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.198 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	22511	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/1548	0.65	0/2087
1	B	0.40	0/1548	0.64	0/2087
1	C	0.41	0/1548	0.63	0/2087
1	D	0.41	0/1548	0.63	0/2087
1	E	0.41	0/1548	0.69	2/2087 (0.1%)
1	F	0.39	0/1548	0.63	0/2087
1	G	0.41	0/1548	0.64	0/2087
1	H	0.42	0/1548	0.63	1/2087 (0.0%)
1	I	0.40	0/1548	0.66	1/2087 (0.0%)
1	J	0.40	0/1548	0.64	0/2087
2	K	0.39	0/690	0.75	5/931 (0.5%)
2	L	0.38	0/690	0.75	5/931 (0.5%)
2	M	0.38	0/690	0.76	5/931 (0.5%)
2	N	0.38	0/690	0.76	5/931 (0.5%)
2	O	0.38	0/690	0.76	5/931 (0.5%)
2	P	0.38	0/690	0.76	5/931 (0.5%)
2	Q	0.40	0/690	0.76	5/931 (0.5%)
2	R	0.40	0/690	0.77	5/931 (0.5%)
2	S	0.41	0/690	0.76	5/931 (0.5%)
2	T	0.39	0/690	0.76	5/931 (0.5%)
All	All	0.40	0/22380	0.68	54/30180 (0.2%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	240	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	E	240	ARG	NE-CZ-NH2	7.99	124.29	120.30
2	R	70	MET	CG-SD-CE	5.92	109.68	100.20
2	K	1	MET	CG-SD-CE	5.91	109.66	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	70	MET	CG-SD-CE	5.91	109.66	100.20

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	1524	0	1543	62	0
1	B	1524	0	1543	54	0
1	C	1524	0	1543	44	0
1	D	1524	0	1543	47	0
1	E	1524	0	1543	57	0
1	F	1524	0	1543	56	0
1	G	1524	0	1543	59	0
1	H	1524	0	1543	55	0
1	I	1524	0	1545	53	0
1	J	1524	0	1543	62	0
2	K	676	0	677	16	0
2	L	676	0	677	18	0
2	M	676	0	677	18	0
2	N	676	0	677	18	0
2	O	676	0	677	23	0
2	P	676	0	677	14	0
2	Q	676	0	677	15	1
2	R	676	0	677	20	0
2	S	676	0	677	19	1
2	T	676	0	677	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1	0	0	1	0
3	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
5	K	12	0	8	2	0
5	M	12	0	8	1	0
5	N	24	0	16	1	0
5	O	12	0	8	1	0
5	P	12	0	8	0	0
5	Q	12	0	8	0	0
5	R	12	0	8	0	0
5	S	12	0	8	1	0
5	T	12	0	8	0	0
6	A	17	0	0	6	0
6	B	18	0	0	1	0
6	C	13	0	0	0	0
6	D	10	0	0	1	0
6	E	13	0	0	0	0
6	F	15	0	0	2	0
6	G	16	0	0	2	0
6	H	21	0	0	1	0
6	I	20	0	0	5	0
6	J	20	0	0	6	0
6	K	17	0	0	2	0
6	L	19	0	0	1	0
6	M	16	0	0	1	0
6	N	16	0	0	1	0
6	O	16	0	0	0	0
6	P	27	0	0	2	0
6	Q	31	0	0	4	0
6	R	28	0	0	0	0
6	S	22	0	0	0	0
6	T	16	0	0	0	0
All	All	22511	0	22282	685	1

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 15.

The worst 5 of 685 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:I:132:CYS:HB3	6:I:3102:HOH:O	1.42	1.17
1:I:148:LEU:HD12	1:I:224:VAL:HG21	1.51	0.91
1:B:148:LEU:HD12	1:B:224:VAL:HG21	1.51	0.90
1:B:59:LEU:HB3	1:B:60:PRO:HD3	1.54	0.90
1:G:148:LEU:HD12	1:G:224:VAL:HG21	1.54	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:45:TYR:OH	2:S:30:GLN:NE2[2_645]	2.07	0.13

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	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
1	B	188/230 (82%)	178 (95%)	8 (4%)	2 (1%)	14	34
1	C	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
1	D	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
1	E	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
1	F	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
1	G	188/230 (82%)	179 (95%)	7 (4%)	2 (1%)	14	34
1	H	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
1	I	188/230 (82%)	178 (95%)	8 (4%)	2 (1%)	14	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	188/230 (82%)	177 (94%)	9 (5%)	2 (1%)	14	34
2	K	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	L	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
2	M	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
2	N	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	O	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
2	P	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	Q	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
2	R	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
2	S	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
2	T	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	2700/3140 (86%)	2560 (95%)	120 (4%)	20 (1%)	22	46

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	B	108	LEU
1	B	110	ASP
1	C	110	ASP
1	D	110	ASP

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	169/196 (86%)	157 (93%)	12 (7%)	14	34
1	B	169/196 (86%)	156 (92%)	13 (8%)	13	30
1	C	169/196 (86%)	158 (94%)	11 (6%)	17	38
1	D	169/196 (86%)	158 (94%)	11 (6%)	17	38
1	E	169/196 (86%)	157 (93%)	12 (7%)	14	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	169/196 (86%)	158 (94%)	11 (6%)	17	38
1	G	169/196 (86%)	158 (94%)	11 (6%)	17	38
1	H	169/196 (86%)	158 (94%)	11 (6%)	17	38
1	I	169/196 (86%)	158 (94%)	11 (6%)	17	38
1	J	169/196 (86%)	157 (93%)	12 (7%)	14	34
2	K	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	L	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	M	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	N	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	O	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	P	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	Q	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	R	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	S	76/76 (100%)	71 (93%)	5 (7%)	16	38
2	T	76/76 (100%)	72 (95%)	4 (5%)	22	48
All	All	2450/2720 (90%)	2286 (93%)	164 (7%)	16	37

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	128	MET
1	H	238	LEU
2	R	43	ASN
1	G	154	LEU
1	H	84	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	61	ASN
1	J	213	ASN
2	S	9	GLN
1	I	150	ASN
1	J	61	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PHE	N	1007	-	9,12,12	0.67	0	10,15,15	0.45	0
5	PHE	R	1002	-	9,12,12	0.74	0	10,15,15	0.54	0
5	PHE	O	1008	-	9,12,12	0.49	0	10,15,15	0.67	1 (10%)
5	PHE	T	1005	-	9,12,12	0.43	0	10,15,15	0.27	0
5	PHE	S	1004	-	9,12,12	0.52	0	10,15,15	0.49	0
5	PHE	N	1006	-	9,12,12	0.50	0	10,15,15	0.43	0
5	PHE	M	1010	-	9,12,12	0.79	0	10,15,15	0.28	0
5	PHE	P	1003	-	9,12,12	0.54	0	10,15,15	0.54	0
5	PHE	K	1009	-	9,12,12	0.41	0	10,15,15	0.27	0
5	PHE	Q	1001	-	9,12,12	0.52	0	10,15,15	0.52	0

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
5	PHE	N	1007	-	-	0/4/8/8	0/1/1/1
5	PHE	R	1002	-	-	1/4/8/8	0/1/1/1
5	PHE	O	1008	-	-	0/4/8/8	0/1/1/1
5	PHE	T	1005	-	-	0/4/8/8	0/1/1/1
5	PHE	S	1004	-	-	0/4/8/8	0/1/1/1
5	PHE	N	1006	-	-	0/4/8/8	0/1/1/1
5	PHE	M	1010	-	-	0/4/8/8	0/1/1/1
5	PHE	P	1003	-	-	0/4/8/8	0/1/1/1
5	PHE	K	1009	-	-	0/4/8/8	0/1/1/1
5	PHE	Q	1001	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1008	PHE	CB-CA-C	-2.04	107.39	110.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	1002	PHE	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1008	PHE	1	0
5	S	1004	PHE	1	0
5	N	1006	PHE	1	0
5	M	1010	PHE	1	0
5	K	1009	PHE	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	192/230 (83%)	0.44	26 (13%) 3 2	18, 38, 89, 107	0
1	B	192/230 (83%)	0.08	13 (6%) 17 15	17, 36, 88, 107	0
1	C	192/230 (83%)	0.14	16 (8%) 11 9	16, 38, 88, 108	0
1	D	192/230 (83%)	0.17	16 (8%) 11 9	18, 39, 89, 108	0
1	E	192/230 (83%)	0.16	12 (6%) 20 19	19, 40, 89, 107	0
1	F	192/230 (83%)	0.18	12 (6%) 20 19	17, 39, 88, 107	0
1	G	192/230 (83%)	0.27	21 (10%) 5 4	16, 39, 88, 108	0
1	H	192/230 (83%)	0.11	12 (6%) 20 19	15, 38, 89, 107	0
1	I	192/230 (83%)	0.12	12 (6%) 20 19	15, 35, 88, 107	0
1	J	192/230 (83%)	0.15	14 (7%) 15 13	16, 38, 90, 108	0
2	K	84/84 (100%)	-0.15	0 100 100	22, 41, 57, 78	0
2	L	84/84 (100%)	-0.21	2 (2%) 59 60	21, 42, 56, 78	0
2	M	84/84 (100%)	-0.08	2 (2%) 59 60	20, 41, 58, 77	0
2	N	84/84 (100%)	0.03	4 (4%) 30 28	21, 41, 58, 79	0
2	O	84/84 (100%)	-0.14	2 (2%) 59 60	21, 41, 59, 78	0
2	P	84/84 (100%)	-0.31	1 (1%) 79 80	18, 40, 58, 78	0
2	Q	84/84 (100%)	-0.17	0 100 100	18, 38, 56, 77	0
2	R	84/84 (100%)	-0.23	2 (2%) 59 60	19, 39, 57, 79	0
2	S	84/84 (100%)	-0.23	1 (1%) 79 80	18, 38, 57, 78	0
2	T	84/84 (100%)	-0.17	3 (3%) 42 42	18, 39, 58, 79	0
All	All	2760/3140 (87%)	0.08	171 (6%) 20 19	15, 39, 84, 108	0

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	109	ASN	10.4
1	J	108	LEU	9.6
1	J	109	ASN	9.4
1	B	108	LEU	9.3
1	F	112	ILE	8.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	D	3108	1/1	0.93	0.07	73,73,73,73	0
5	PHE	N	1007	12/12	0.94	0.16	33,35,37,38	0
3	ZN	I	3101	1/1	0.95	0.08	50,50,50,50	0
3	ZN	E	3105	1/1	0.96	0.03	57,57,57,57	0
5	PHE	M	1010	12/12	0.96	0.12	21,24,26,28	0
5	PHE	Q	1001	12/12	0.96	0.12	18,21,25,28	0
4	K	K	2006	1/1	0.96	0.05	27,27,27,27	0
5	PHE	N	1006	12/12	0.96	0.12	24,28,29,30	0
5	PHE	R	1002	12/12	0.96	0.14	19,21,23,24	0
4	K	Q	2005	1/1	0.97	0.08	23,23,23,23	0
5	PHE	K	1009	12/12	0.97	0.10	17,21,25,26	0
5	PHE	O	1008	12/12	0.97	0.10	21,23,24,25	0
3	ZN	B	3109	1/1	0.97	0.04	54,54,54,54	0
4	K	O	2010	1/1	0.97	0.09	35,35,35,35	0
5	PHE	P	1003	12/12	0.97	0.10	18,20,25,26	0
4	K	N	2009	1/1	0.97	0.08	36,36,36,36	0
3	ZN	J	3106	1/1	0.97	0.05	53,53,53,53	0
5	PHE	T	1005	12/12	0.98	0.10	16,18,21,24	0
4	K	R	2001	1/1	0.98	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	K	M	2008	1/1	0.98	0.05	32,32,32,32	0
4	K	L	2007	1/1	0.98	0.06	29,29,29,29	0
3	ZN	A	3102	1/1	0.98	0.05	53,53,53,53	0
5	PHE	S	1004	12/12	0.98	0.08	9,13,15,17	0
4	K	S	2002	1/1	0.98	0.07	23,23,23,23	0
3	ZN	G	3103	1/1	0.99	0.04	56,56,56,56	0
3	ZN	H	3104	1/1	0.99	0.04	49,49,49,49	0
3	ZN	F	3110	1/1	0.99	0.03	62,62,62,62	0
3	ZN	C	3107	1/1	0.99	0.06	55,55,55,55	0
4	K	T	2003	1/1	0.99	0.08	30,30,30,30	0
4	K	P	2004	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.