



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 10:07 AM BST

PDB ID : 1IS7  
Title : Crystal structure of rat GTPCHI/GFRP stimulatory complex  
Authors : Maita, N.; Okada, K.; Hatakeyama, K.; Hakoshima, T.  
Deposited on : 2001-11-18  
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.

---

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

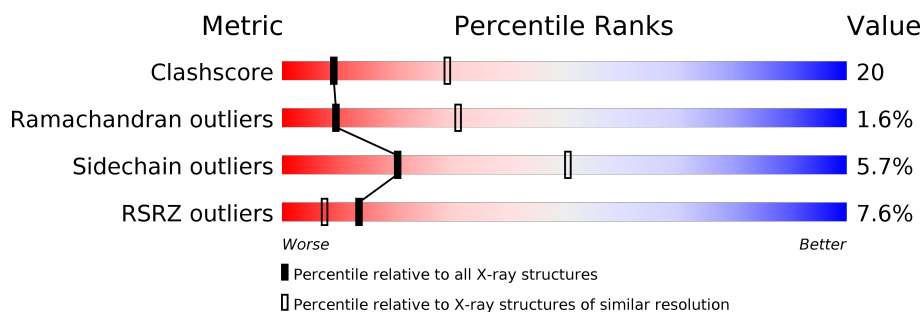
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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>9%</div> <div>53% 26% 16%</div> </div>
1	B	230	<div> <div>10%</div> <div>56% 25% 16%</div> </div>
1	C	230	<div> <div>12%</div> <div>53% 27% 16%</div> </div>
1	D	230	<div> <div>4%</div> <div>56% 24% 16%</div> </div>
1	E	230	<div> <div>9%</div> <div>55% 26% 16%</div> </div>
1	F	230	<div> <div>6%</div> <div>54% 25% 16%</div> </div>
1	G	230	<div> <div>6%</div> <div>56% 24% 16%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
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 5 unique types of molecules in this entry. The entry contains 22375 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
			1536	967	271	287	11			
1	B	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	C	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	D	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	E	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	F	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	G	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	H	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	I	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	J	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	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			

*Continued on next page...*

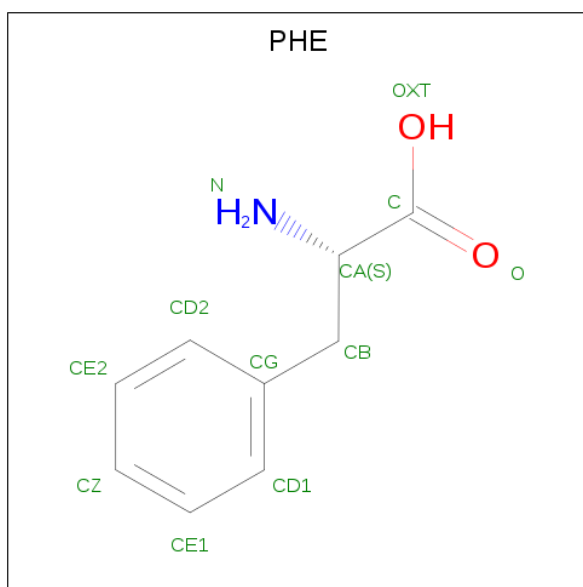
*Continued from previous page...*

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	K	1	Total	C	N	O	0	0
			12	9	1	2		
4	L	1	Total	C	N	O	0	0
			12	9	1	2		
4	M	1	Total	C	N	O	0	0
			12	9	1	2		
4	N	1	Total	C	N	O	0	0
			12	9	1	2		
4	O	1	Total	C	N	O	0	0
			12	9	1	2		
4	P	1	Total	C	N	O	0	0
			12	9	1	2		
4	R	1	Total	C	N	O	0	0
			12	9	1	2		
4	R	1	Total	C	N	O	0	0
			12	9	1	2		
4	S	1	Total	C	N	O	0	0
			12	9	1	2		
4	T	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	4	Total	O	0	0
			4	4		

*Continued on next page...*

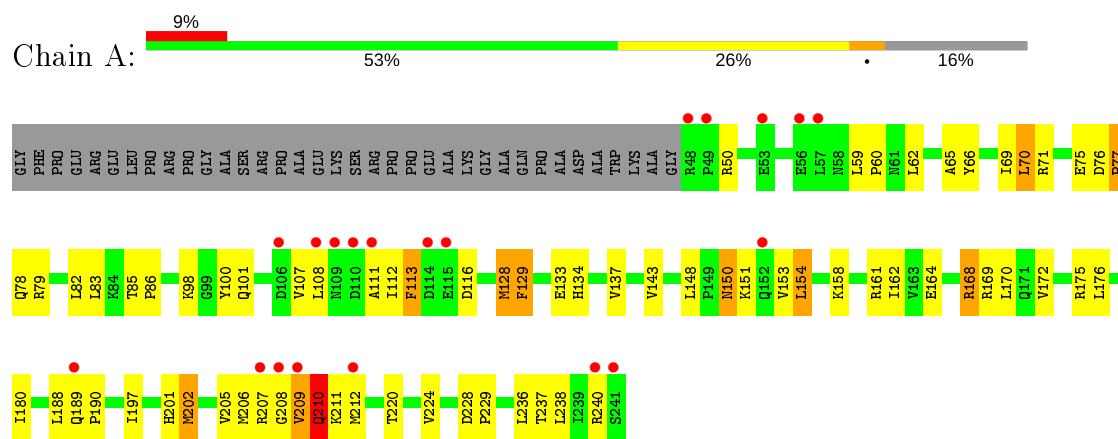
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	5	Total 5	O 5	0	0
5	D	4	Total 4	O 4	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0
5	G	9	Total 9	O 9	0	0
5	H	5	Total 5	O 5	0	0
5	I	3	Total 3	O 3	0	0
5	J	4	Total 4	O 4	0	0
5	K	8	Total 8	O 8	0	0
5	L	9	Total 9	O 9	0	0
5	N	9	Total 9	O 9	0	0
5	O	9	Total 9	O 9	0	0
5	P	12	Total 12	O 12	0	0
5	Q	9	Total 9	O 9	0	0
5	R	6	Total 6	O 6	0	0
5	S	7	Total 7	O 7	0	0
5	T	7	Total 7	O 7	0	0

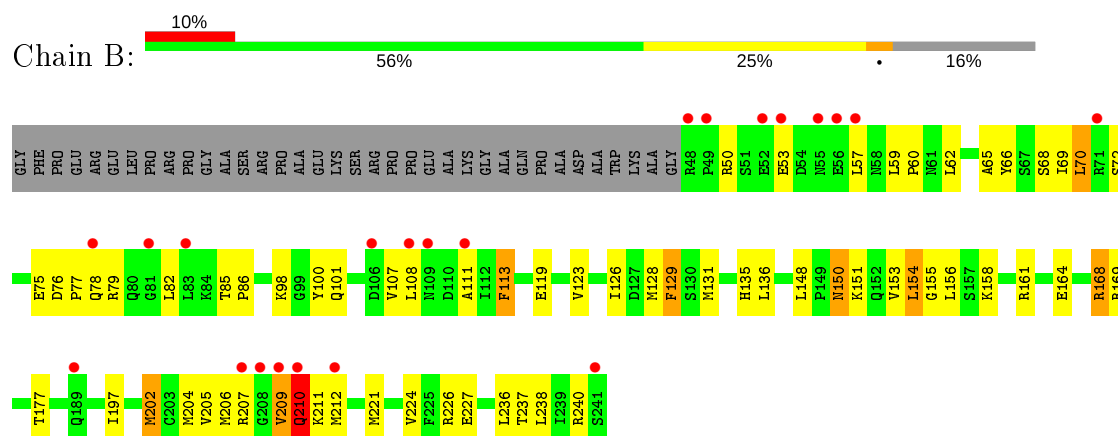
### 3 Residue-property plots [i](#)

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.

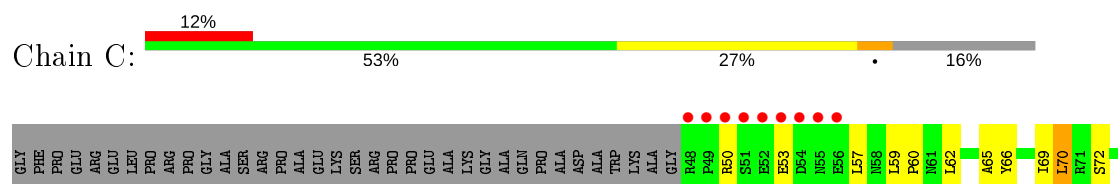
#### • Molecule 1: GTP Cyclohydrolase I



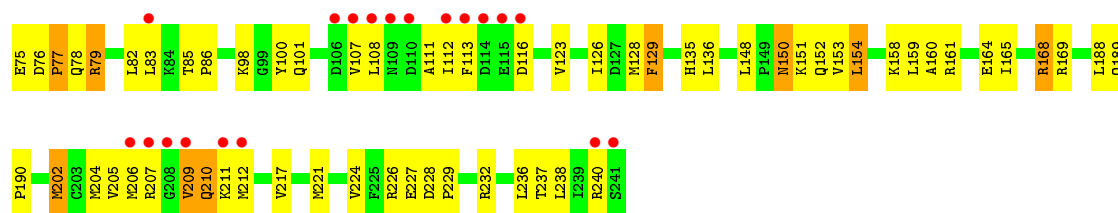
#### • Molecule 1: GTP Cyclohydrolase I



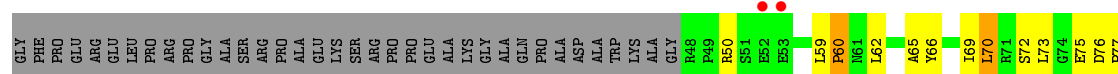
#### • Molecule 1: GTP Cyclohydrolase I



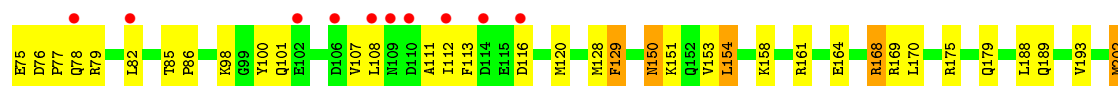
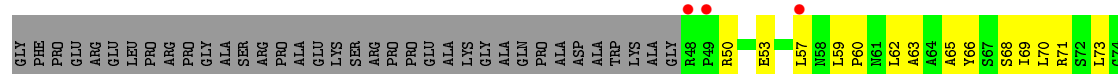




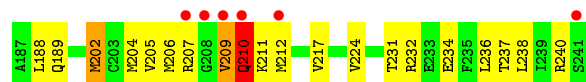
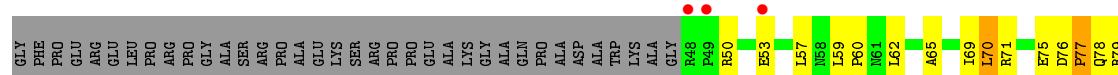
• Molecule 1: GTP Cyclohydrolase I



• Molecule 1: GTP Cyclohydrolase I



• Molecule 1: GTP Cyclohydrolase I



Chain G:

Position	Amino Acid	Frequency (%)
1	GLY	6%
2	GLY	56%
3	GLY	24%
4	GLY	16%

Chain H:

Sequence logo for Chain H. The y-axis represents information content in bits (0.00 to 0.10). The x-axis shows positions 1 to 241. A color scale at the top indicates conservation levels: 8% (red), 56% (green), 24% (yellow), and 16% (grey).

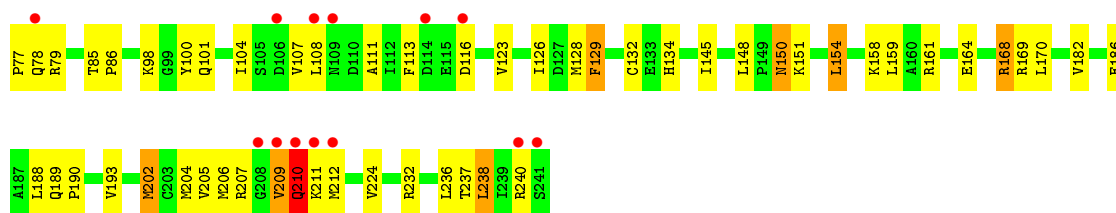
Conserved residues (high information content) are highlighted in red and yellow. Key residues include:

- Position 1: D76
- Position 2: P77
- Position 3: Q78
- Position 4: R79
- Position 5: L82
- Position 6: T85
- Position 7: P86
- Position 8: K98
- Position 9: G99
- Position 10: Y100
- Position 11: Q101
- Position 12: E102
- Position 13: T103
- Position 14: I104
- Position 15: S105
- Position 16: D106
- Position 17: V107
- Position 18: L108
- Position 19: N109
- Position 20: D110
- Position 21: A111
- Position 22: I112
- Position 23: F113
- Position 24: D114
- Position 25: E115
- Position 26: D116
- Position 27: M120
- Position 28: M128
- Position 29: F129
- Position 30: V137
- Position 31: Y143
- Position 32: L148
- Position 33: P149
- Position 34: N150
- Position 35: K151
- Position 36: Q152
- Position 37: L153
- Position 38: A154
- Position 39: G155
- Position 40: K159
- Position 41: R161
- Position 42: R168
- Position 43: R169
- Position 44: L188
- Position 45: Q189
- Position 46: V202
- Position 47: G203
- Position 48: M204
- Position 49: V205
- Position 50: V206
- Position 51: R207
- Position 52: G208
- Position 53: V209
- Position 54: Q210
- Position 55: K211
- Position 56: M212
- Position 57: N213
- Position 58: S214
- Position 59: K215
- Position 60: V224
- Position 61: D228
- Position 62: P229
- Position 63: K230
- Position 64: T231
- Position 65: L236
- Position 66: T237
- Position 67: L238
- Position 68: F239
- Position 69: R240
- Position 70: S241

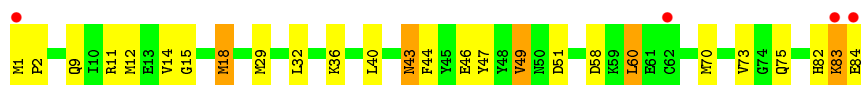
Chain I:

10%	54%	25%	16%
GLY	PRO	ARG	GLY
PHE	ARG	GLY	ALA
PRO	ALA	SER	SER
GLU	ARG	ARG	ARG
GLU	PRO	PRO	PRO
LEU	ALA	ALA	ALA
PRO	GLU	GLU	GLU
ARG	LYS	LYS	LYS
PRO	SER	SER	SER
GLY	ARG	ARG	ARG
ALA	PRO	PRO	PRO
SER	ALA	ALA	ALA
ARG	GLY	GLY	GLY
PRO	LYS	LYS	LYS
GLU	SER	SER	SER
LYS	ARG	ARG	ARG
ALA	PRO	PRO	PRO
GLY	ALA	ALA	ALA
LYS	GLY	GLY	GLY
ALA	GLN	GLN	GLN
GLY	ALA	ALA	ALA
ASP	ASP	ASP	ASP
ALA	ALA	ALA	ALA
TRP	TRP	TRP	TRP
LYS	LYS	LYS	LYS
ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY
R48	R49	R50	R51
P49	P50	P51	P52
R50	R51	R52	R53
S51	S52	S53	S54
E53	E54	E55	E56
D54	D55	D56	D57
N55	N56	N57	N58
E56	E57	E58	E59
L57	L58	L59	L60
N58	N59	N60	N61
L59	L60	L61	L62
P60	P61	P62	P63
R61	R62	R63	R64
E64	E65	E66	E67
R65	R66	R67	R68
L66	L67	L68	L69
N68	N69	N70	N71
E69	E70	E71	E72
R70	R71	R72	R73
L71	L72	L73	L74
N72	N73	N74	N75
E73	E74	E75	E76
R74	R75	R76	R77
L75	L76	L77	L78
N76	N77	N78	N79
E76	E77	E78	E79
R77	R78	R79	R80
L78	L79	L80	L81
N79	N80	N81	N82
E79	E80	E81	E82
R80	R81	R82	R83
L81	L82	L83	L84
N82	N83	N84	N85
E82	E83	E84	E85
R83	R84	R85	R86
L84	L85	L86	L87
N85	N86	N87	N88
E85	E86	E87	E88
R86	R87	R88	R89
L87	L88	L89	L90
N88	N89	N90	N91
E88	E89	E90	E91
R89	R90	R91	R92
L90	L91	L92	L93
N91	N92	N93	N94
E91	E92	E93	E94
R92	R93	R94	R95
L93	L94	L95	L96
N94	N95	N96	N97
E94	E95	E96	E97
R95	R96	R97	R98
L96	L97	L98	L99
N97	N98	N99	N100
E97	E98	E99	E100
R98	R99	R100	R101
L99	L100	L101	L102
N100	N101	N102	N103
E100	E101	E102	E103
R101	R102	R103	R104
L102	L103	L104	L105
N103	N104	N105	N106
E103	E104	E105	E106
R104	R105	R106	R107
L105	L106	L107	L108
N106	N107	N108	N109
E106	E107	E108	E109
R107	R108	R109	R110
L108	L109	L110	L111
N109	N110	N111	N112
E109	E110	E111	E112
R110	R111	R112	R113
L111	L112	L113	L114
N112	N113	N114	N115
E112	E113	E114	E115
R113	R114	R115	R116
L114	L115	L116	L117
N115	N116	N117	N118
E115	E116	E117	E118
R116	R117	R118	R119
L117	L118	L119	L120
N118	N119	N120	N121
E118	E119	E120	E121
R119	R120	R121	R122
L120	L121	L122	L123
N121	N122	N123	N124
E121	E122	E123	E124
R122	R123	R124	R125
L123	L124	L125	L126
N124	N125	N126	

Chain J:   
 GLY PHE PRO GLU ARG GLU LEU PRO ARG GLY ALA SER ARG PRO ALA GLU LYS SER ARG PRO PRO GLU LYS ALA ASP TRP LYS ALA GLY ARG P49 R50 E53 D54 D55 L57 N58 L59 P60 A63 A64 A65 I69 L70 R71 S72 E75 D76



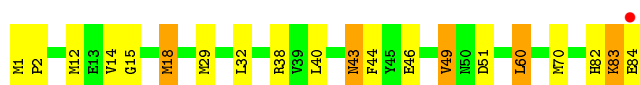
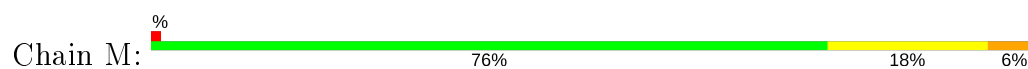
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



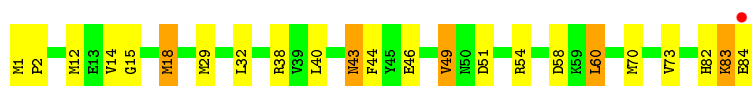
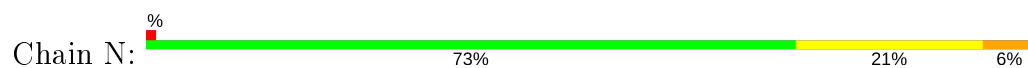
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



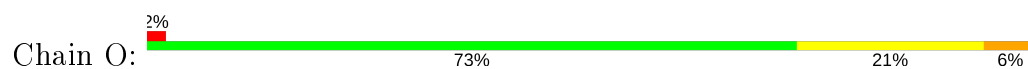
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

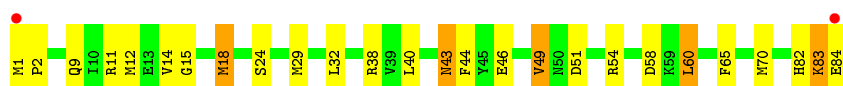


● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

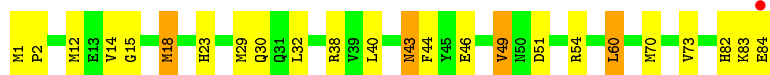


● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

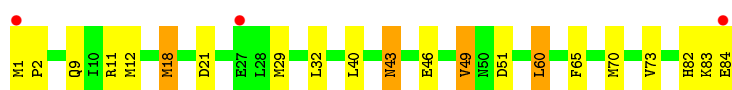
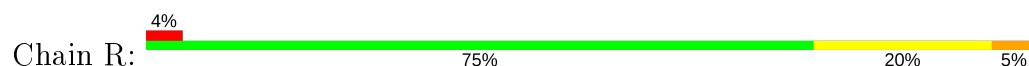




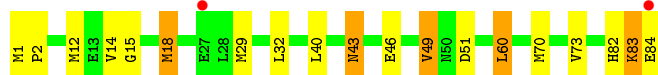
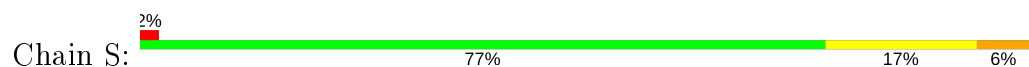
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



● 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, $\alpha$ , $\beta$ , $\gamma$	124.15Å 111.72Å 126.11Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.80) 99.2 (15.00-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.51Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.228 , 0.264 0.240 , (Not available)	Depositor DCC
$R_{free}$ test set	33257 reflections (28.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 31.50 % 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 1.0964e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	0.42	0/1561	0.64	0/2107
1	B	0.43	0/1561	0.63	0/2107
1	C	0.44	0/1561	0.64	0/2107
1	D	0.43	0/1561	0.65	0/2107
1	E	0.44	0/1561	0.65	0/2107
1	F	0.43	0/1561	0.63	0/2107
1	G	0.44	0/1561	0.64	0/2107
1	H	0.44	0/1561	0.65	0/2107
1	I	0.44	0/1561	0.63	0/2107
1	J	0.43	0/1561	0.65	0/2107
2	K	0.40	0/690	0.77	5/931 (0.5%)
2	L	0.40	0/690	0.76	5/931 (0.5%)
2	M	0.42	0/690	0.77	5/931 (0.5%)
2	N	0.47	1/690 (0.1%)	0.74	4/931 (0.4%)
2	O	0.41	0/690	0.75	5/931 (0.5%)
2	P	0.42	0/690	0.77	5/931 (0.5%)
2	Q	0.42	0/690	0.77	5/931 (0.5%)
2	R	0.41	0/690	0.76	5/931 (0.5%)
2	S	0.39	0/690	0.76	5/931 (0.5%)
2	T	0.41	0/690	0.77	5/931 (0.5%)
All	All	0.43	1/22510 (0.0%)	0.68	49/30380 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	29	MET	CG-SD	5.74	1.96	1.81

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	MET	CG-SD-CE	6.04	109.87	100.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	29	MET	CG-SD-CE	6.00	109.80	100.20
2	S	29	MET	CG-SD-CE	5.99	109.78	100.20
2	O	29	MET	CG-SD-CE	5.97	109.75	100.20
2	K	1	MET	CG-SD-CE	5.96	109.74	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	1536	0	1557	81	0
1	B	1536	0	1557	88	0
1	C	1536	0	1557	84	0
1	D	1536	0	1557	83	0
1	E	1536	0	1557	83	0
1	F	1536	0	1557	87	0
1	G	1536	0	1557	83	0
1	H	1536	0	1557	79	0
1	I	1536	0	1557	85	0
1	J	1536	0	1557	76	0
2	K	676	0	677	20	0
2	L	676	0	677	21	0
2	M	676	0	677	15	0
2	N	676	0	677	18	0
2	O	676	0	677	20	0
2	P	676	0	677	22	0
2	Q	676	0	677	18	1
2	R	676	0	677	16	0
2	S	676	0	677	15	0
2	T	676	0	677	19	1
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
4	K	12	0	8	1	0
4	L	12	0	8	1	0
4	M	12	0	8	0	0
4	N	12	0	8	0	0
4	O	12	0	8	0	0
4	P	12	0	8	0	0
4	R	24	0	16	0	0
4	S	12	0	8	0	0
4	T	12	0	8	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
5	C	5	0	0	1	0
5	D	4	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	9	0	0	1	0
5	H	5	0	0	0	0
5	I	3	0	0	0	0
5	J	4	0	0	0	0
5	K	8	0	0	1	0
5	L	9	0	0	2	0
5	N	9	0	0	0	0
5	O	9	0	0	0	0
5	P	12	0	0	0	0
5	Q	9	0	0	0	0
5	R	6	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
All	All	22375	0	22420	893	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 20.

The worst 5 of 893 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:HB3	1:I:210:GLN:HB3	1.27	1.14
1:A:205:VAL:HG22	1:A:212:MET:HA	1.42	1.01
1:H:205:VAL:HG13	1:H:212:MET:HB2	1.41	1.01
1:J:209:VAL:HG13	1:J:210:GLN:H	1.25	1.00
1:I:205:VAL:HG13	1:I:212:MET:HB2	1.41	1.00

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:30:GLN:NE2	2:T:45:TYR:OH[2_556]	2.01	0.19

## 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%)	171 (89%)	17 (9%)	4 (2%)	7	23
1	B	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	9	31
1	C	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	7	23
1	D	192/230 (84%)	171 (89%)	18 (9%)	3 (2%)	9	31
1	E	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	9	31
1	F	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	7	23
1	G	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	9	31
1	H	192/230 (84%)	172 (90%)	15 (8%)	5 (3%)	5	18
1	I	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	7	23
1	J	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	9	31
2	K	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	L	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	M	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	O	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	P	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	Q	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	R	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	S	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	T	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	2740/3140 (87%)	2475 (90%)	222 (8%)	43 (2%)	9	31

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	209	VAL
1	B	108	LEU
1	B	209	VAL
1	C	108	LEU

### 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%)	160 (94%)	10 (6%)	19	49
1	B	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	C	170/196 (87%)	159 (94%)	11 (6%)	17	44
1	D	170/196 (87%)	159 (94%)	11 (6%)	17	44
1	E	170/196 (87%)	161 (95%)	9 (5%)	22	54
1	F	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	G	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	H	170/196 (87%)	159 (94%)	11 (6%)	17	44
1	I	170/196 (87%)	160 (94%)	10 (6%)	19	49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	170/196 (87%)	161 (95%)	9 (5%)	22	54
2	K	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	L	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	M	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	N	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	O	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	P	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	Q	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	R	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	S	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	T	76/76 (100%)	72 (95%)	4 (5%)	22	54
All	All	2460/2720 (90%)	2319 (94%)	141 (6%)	20	50

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	128	MET
1	H	202	MET
2	R	43	ASN
1	G	150	ASN
1	H	70	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	150	ASN
2	K	43	ASN
2	S	43	ASN
1	I	213	ASN
1	J	134	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 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	$\# Z  > 2$
4	PHE	R	1002	-	9,12,12	0.47	0	10,15,15	0.35	0
4	PHE	O	1008	-	9,12,12	0.50	0	10,15,15	0.50	0
4	PHE	S	1004	-	9,12,12	0.37	0	10,15,15	0.29	0
4	PHE	P	1003	-	9,12,12	0.50	0	10,15,15	0.42	0
4	PHE	M	1006	-	9,12,12	0.43	0	10,15,15	0.25	0
4	PHE	L	1010	-	9,12,12	0.53	0	10,15,15	0.65	0
4	PHE	N	1007	-	9,12,12	0.57	0	10,15,15	0.39	0
4	PHE	K	1009	-	9,12,12	0.54	0	10,15,15	0.61	0
4	PHE	T	1005	-	9,12,12	0.50	0	10,15,15	0.59	0
4	PHE	R	1001	-	9,12,12	0.46	0	10,15,15	0.44	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
4	PHE	R	1002	-	-	3/4/8/8	0/1/1/1
4	PHE	O	1008	-	-	0/4/8/8	0/1/1/1
4	PHE	S	1004	-	-	1/4/8/8	0/1/1/1
4	PHE	P	1003	-	-	0/4/8/8	0/1/1/1
4	PHE	M	1006	-	-	0/4/8/8	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PHE	L	1010	-	-	0/4/8/8	0/1/1/1
4	PHE	N	1007	-	-	0/4/8/8	0/1/1/1
4	PHE	K	1009	-	-	0/4/8/8	0/1/1/1
4	PHE	T	1005	-	-	0/4/8/8	0/1/1/1
4	PHE	R	1001	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	1002	PHE	N-CA-CB-CG
4	S	1004	PHE	N-CA-CB-CG
4	R	1002	PHE	CA-CB-CG-CD1
4	R	1002	PHE	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1010	PHE	1	0
4	K	1009	PHE	1	0

## 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%)	0.06	20 (10%) 6 3	21, 53, 102, 110	0
1	B	194/230 (84%)	0.16	22 (11%) 5 3	22, 55, 101, 110	0
1	C	194/230 (84%)	0.32	28 (14%) 2 1	20, 52, 102, 111	0
1	D	194/230 (84%)	-0.06	10 (5%) 27 18	17, 50, 101, 110	0
1	E	194/230 (84%)	0.06	20 (10%) 6 3	17, 54, 101, 110	0
1	F	194/230 (84%)	0.01	14 (7%) 15 8	17, 53, 102, 111	0
1	G	194/230 (84%)	0.03	14 (7%) 15 8	17, 50, 101, 110	0
1	H	194/230 (84%)	0.11	19 (9%) 7 4	17, 53, 102, 110	0
1	I	194/230 (84%)	0.23	24 (12%) 4 2	21, 56, 101, 110	0
1	J	194/230 (84%)	0.05	17 (8%) 10 5	20, 53, 102, 111	0
2	K	84/84 (100%)	-0.10	4 (4%) 30 21	24, 51, 71, 90	0
2	L	84/84 (100%)	-0.10	5 (5%) 21 14	24, 53, 72, 91	0
2	M	84/84 (100%)	-0.12	1 (1%) 79 73	24, 52, 71, 91	0
2	N	84/84 (100%)	-0.29	1 (1%) 79 73	25, 52, 70, 90	0
2	O	84/84 (100%)	-0.27	2 (2%) 59 49	23, 51, 70, 90	0
2	P	84/84 (100%)	-0.17	2 (2%) 59 49	23, 50, 70, 89	0
2	Q	84/84 (100%)	-0.20	1 (1%) 79 73	22, 50, 68, 89	0
2	R	84/84 (100%)	-0.17	3 (3%) 42 32	24, 50, 71, 90	0
2	S	84/84 (100%)	-0.22	2 (2%) 59 49	21, 52, 70, 89	0
2	T	84/84 (100%)	-0.10	2 (2%) 59 49	23, 50, 71, 90	0
All	All	2780/3140 (88%)	0.02	211 (7%) 13 7	17, 52, 100, 111	0

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	ASN	12.6
1	B	109	ASN	8.1
1	H	109	ASN	7.6
1	G	108	LEU	7.0
1	E	109	ASN	6.8

## 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 monosaccharides 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
3	K	R	2001	1/1	0.91	0.10	56,56,56,56	0
3	K	S	2002	1/1	0.92	0.09	53,53,53,53	0
3	K	O	2010	1/1	0.93	0.09	52,52,52,52	0
4	PHE	K	1009	12/12	0.94	0.15	37,40,43,43	0
4	PHE	O	1008	12/12	0.95	0.14	28,33,34,34	0
3	K	L	2007	1/1	0.95	0.07	48,48,48,48	0
4	PHE	R	1001	12/12	0.96	0.13	17,21,23,25	0
4	PHE	N	1007	12/12	0.96	0.13	20,24,26,28	0
3	K	M	2008	1/1	0.96	0.07	43,43,43,43	0
3	K	Q	2005	1/1	0.96	0.05	39,39,39,39	0
4	PHE	R	1002	12/12	0.96	0.13	25,29,33,34	0
3	K	K	2006	1/1	0.97	0.05	48,48,48,48	0
4	PHE	M	1006	12/12	0.97	0.10	23,27,30,32	0
3	K	N	2009	1/1	0.97	0.06	42,42,42,42	0
4	PHE	S	1004	12/12	0.97	0.12	17,22,26,28	0
4	PHE	P	1003	12/12	0.97	0.13	26,27,29,30	0
4	PHE	T	1005	12/12	0.97	0.12	24,28,32,33	0
4	PHE	L	1010	12/12	0.97	0.13	28,30,31,35	0
3	K	P	2004	1/1	0.97	0.07	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	T	2003	1/1	0.98	0.06	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.