Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 07:35 PM GMT

PDB ID	:	4UQF
Title	:	CRYSTAL STRUCTURE OF LISTERIA MONOCYTOGENES GTP CYCLOHYDROLASE I
Authors	:	Schuessler, S.; Perbandt, M.; Fischer, M.; Graewert, T.
Deposited on	:	2014-06-23
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

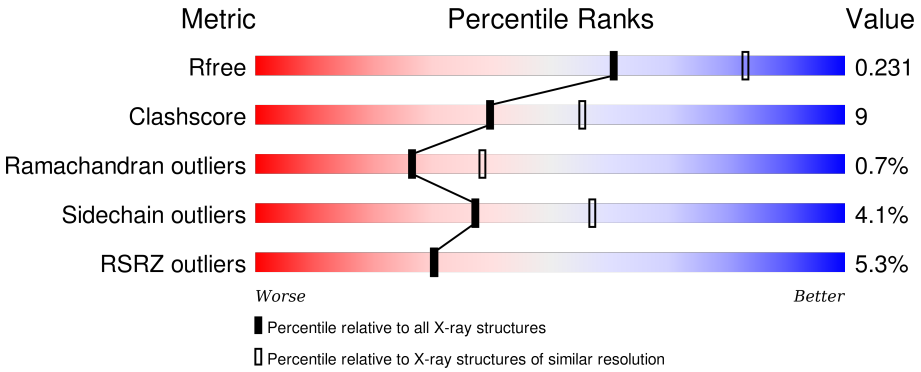
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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 <=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	202	2% 77% 14% 8%
1	B	202	4% 76% 15% 8%
1	C	202	2% 77% 13% • 8%
1	D	202	7% 76% 15% 8%
1	E	202	4% 72% 18% • 8%

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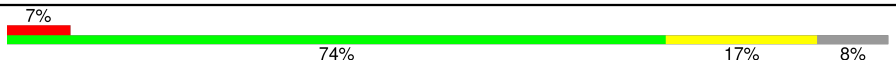
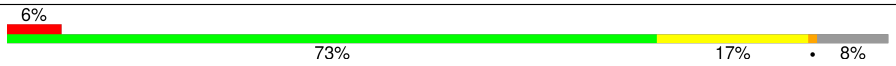
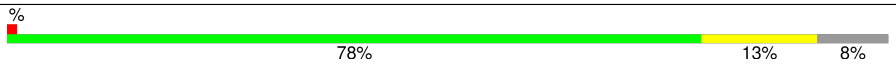
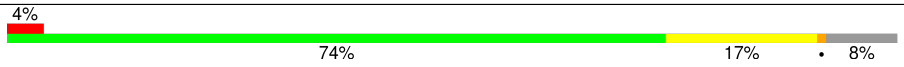
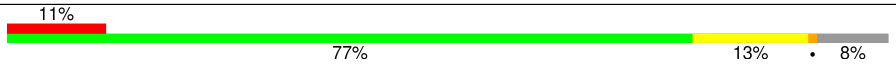
Mol	Chain	Length	Quality of chain
1	F	202	
1	G	202	
1	H	202	
1	I	202	
1	J	202	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14475 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1458	922	258	267	11			
1	B	186	Total	C	N	O	S	0	0	0
			1437	909	256	261	11			
1	C	186	Total	C	N	O	S	0	0	0
			1461	923	259	268	11			
1	D	186	Total	C	N	O	S	0	0	0
			1465	926	260	268	11			
1	E	186	Total	C	N	O	S	0	0	0
			1449	916	256	266	11			
1	F	186	Total	C	N	O	S	0	0	0
			1438	907	257	263	11			
1	G	186	Total	C	N	O	S	0	0	0
			1415	890	251	263	11			
1	H	186	Total	C	N	O	S	0	0	0
			1458	922	258	267	11			
1	I	186	Total	C	N	O	S	0	0	0
			1441	910	255	265	11			
1	J	186	Total	C	N	O	S	0	0	0
			1453	916	259	267	11			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
A	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
A	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
A	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
A	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
A	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
A	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
A	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
A	-4	SER	-	EXPRESSION TAG	UNP W6E2R7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
A	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
A	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
A	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
A	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
B	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
B	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
B	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
B	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
B	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
B	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
B	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
B	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
B	-4	SER	-	EXPRESSION TAG	UNP W6E2R7
B	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
B	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
B	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
B	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
B	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
C	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
C	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
C	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
C	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
C	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
C	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
C	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
C	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
C	-4	SER	-	EXPRESSION TAG	UNP W6E2R7
C	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
C	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
C	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
C	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
C	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
D	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
D	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
D	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
D	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
D	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
D	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
D	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
D	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
D	-4	SER	-	EXPRESSION TAG	UNP W6E2R7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
D	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
D	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
D	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
D	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
E	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
E	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
E	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
E	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
E	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
E	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
E	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
E	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
E	-4	SER	-	EXPRESSION TAG	UNP W6E2R7
E	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
E	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
E	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
E	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
E	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
F	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
F	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
F	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
F	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
F	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
F	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
F	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
F	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
F	-4	SER	-	EXPRESSION TAG	UNP W6E2R7
F	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
F	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
F	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
F	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
F	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
G	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
G	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
G	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
G	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
G	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
G	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
G	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
G	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
G	-4	SER	-	EXPRESSION TAG	UNP W6E2R7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
G	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
G	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
G	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
G	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
H	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
H	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
H	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
H	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
H	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
H	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
H	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
H	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
H	-4	SER	-	EXPRESSION TAG	UNP W6E2R7
H	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
H	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
H	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
H	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
H	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
I	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
I	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
I	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
I	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
I	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
I	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
I	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
I	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
I	-4	SER	-	EXPRESSION TAG	UNP W6E2R7
I	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
I	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
I	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
I	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
I	1	LYS	-	EXPRESSION TAG	UNP W6E2R7
J	-12	MET	-	EXPRESSION TAG	UNP W6E2R7
J	-11	HIS	-	EXPRESSION TAG	UNP W6E2R7
J	-10	HIS	-	EXPRESSION TAG	UNP W6E2R7
J	-9	HIS	-	EXPRESSION TAG	UNP W6E2R7
J	-8	HIS	-	EXPRESSION TAG	UNP W6E2R7
J	-7	HIS	-	EXPRESSION TAG	UNP W6E2R7
J	-6	HIS	-	EXPRESSION TAG	UNP W6E2R7
J	-5	GLY	-	EXPRESSION TAG	UNP W6E2R7
J	-4	SER	-	EXPRESSION TAG	UNP W6E2R7

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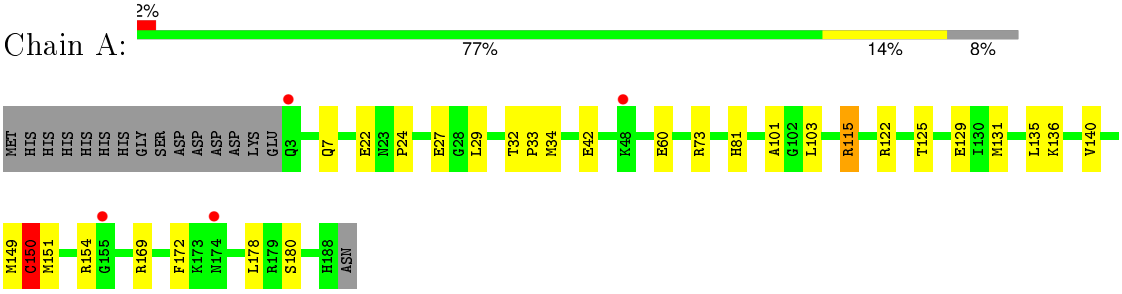
Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	ASP	-	EXPRESSION TAG	UNP W6E2R7
J	-2	ASP	-	EXPRESSION TAG	UNP W6E2R7
J	-1	ASP	-	EXPRESSION TAG	UNP W6E2R7
J	0	ASP	-	EXPRESSION TAG	UNP W6E2R7
J	1	LYS	-	EXPRESSION TAG	UNP W6E2R7

3 Residue-property plots (i)

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

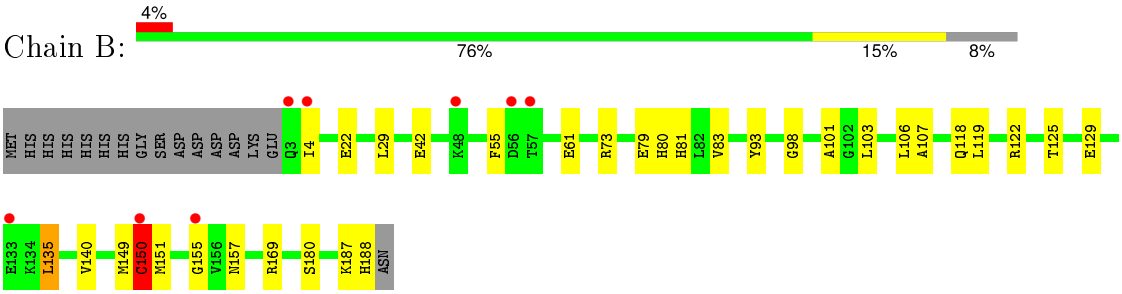
- Molecule 1: GTP CYCLOHYDROLASE 1

Chain A:



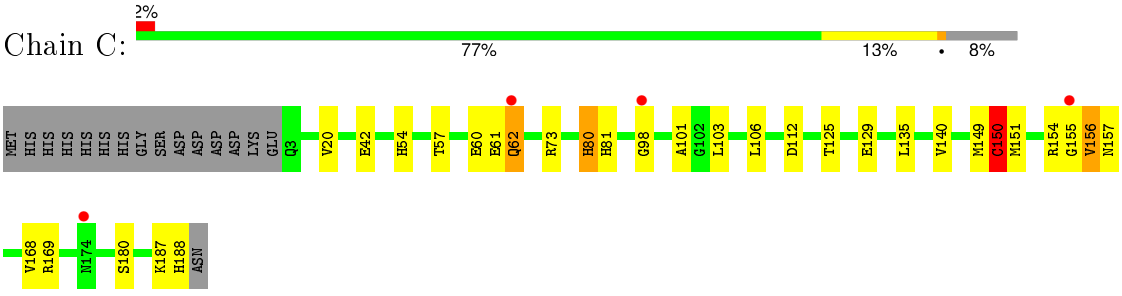
- Molecule 1: GTP CYCLOHYDROLASE 1

Chain B:



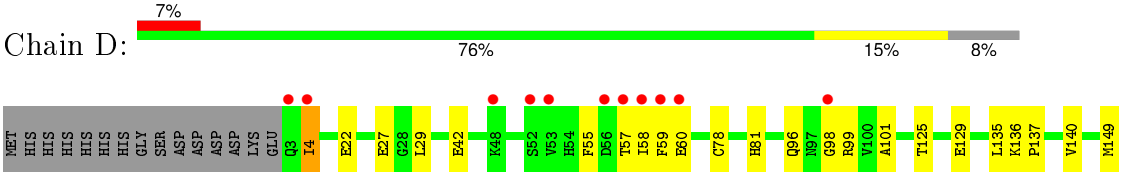
- Molecule 1: GTP CYCLOHYDROLASE 1

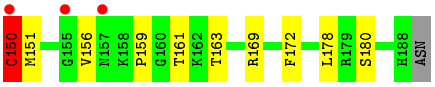
Chain C:



- Molecule 1: GTP CYCLOHYDROLASE 1

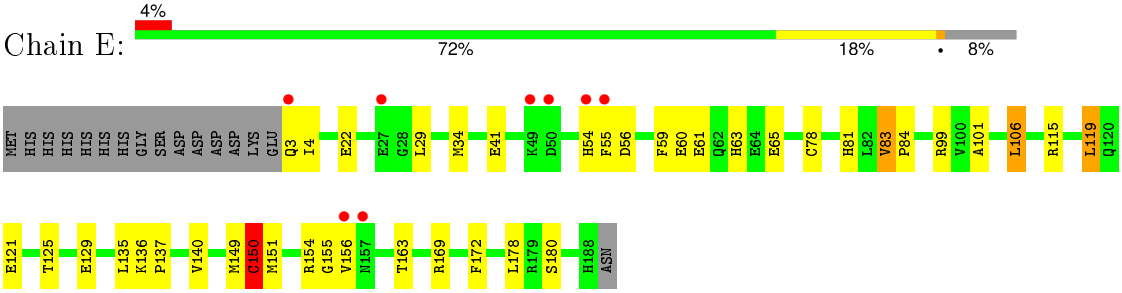
Chain D:





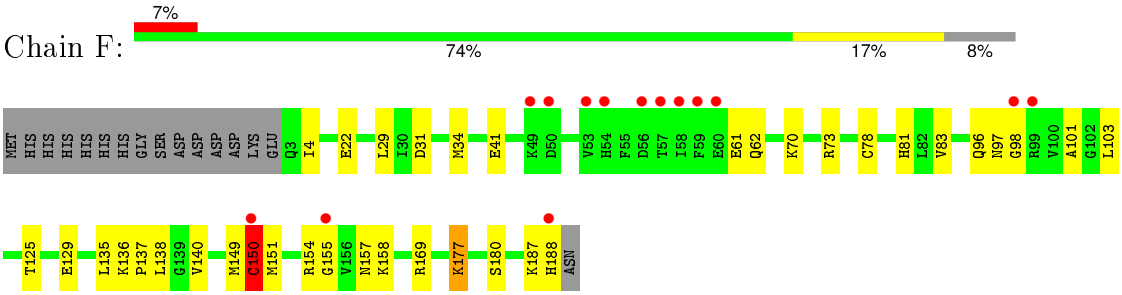
• Molecule 1: GTP CYCLOHYDROLASE 1

Chain E:



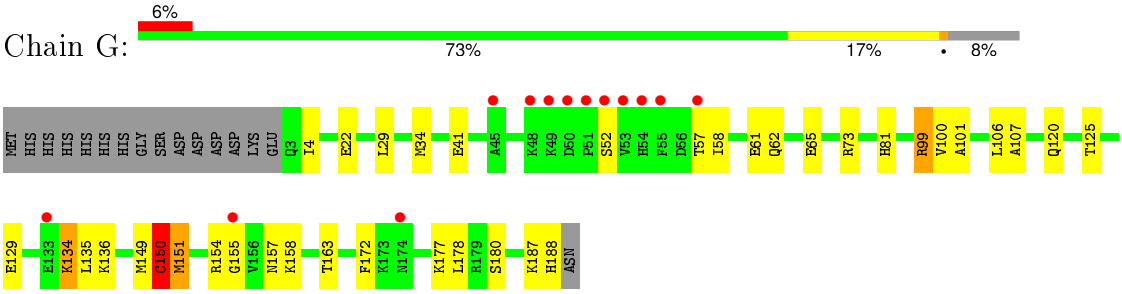
• Molecule 1: GTP CYCLOHYDROLASE 1

Chain F:



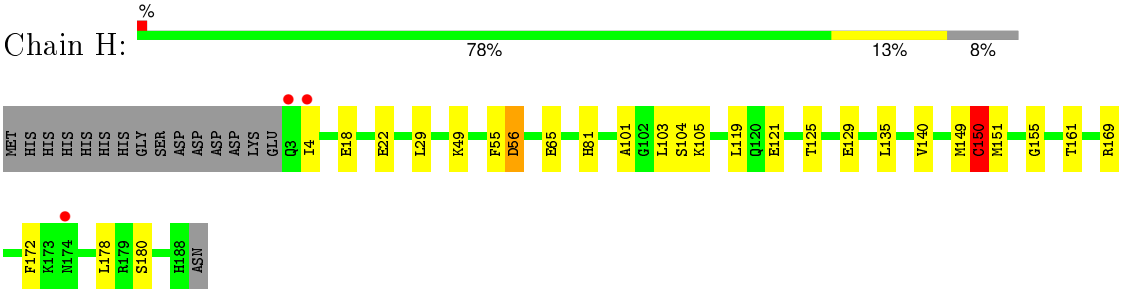
• Molecule 1: GTP CYCLOHYDROLASE 1

Chain G:



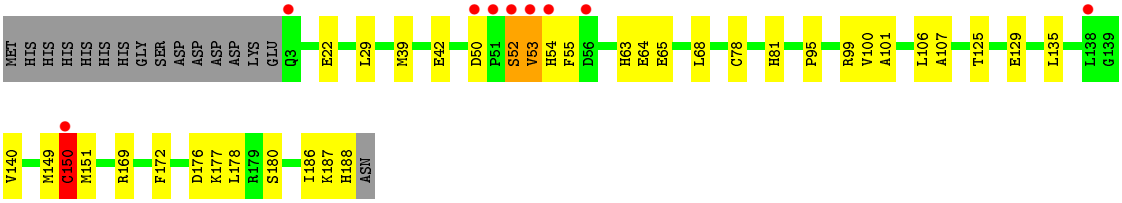
• Molecule 1: GTP CYCLOHYDROLASE 1

Chain H:

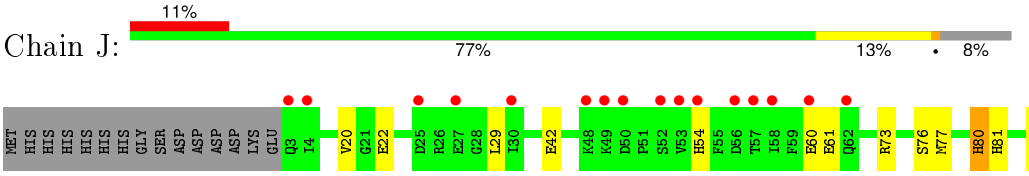


• Molecule 1: GTP CYCLOHYDROLASE 1

Chain I:



• Molecule 1: GTP CYCLOHYDROLASE 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.25Å 141.85Å 90.78Å 90.00° 104.61° 90.00°	Depositor
Resolution (Å)	87.84 – 2.40 29.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (87.84-2.40) 99.7 (29.99-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.192 , 0.226 0.205 , 0.231	Depositor DCC
R_{free} test set	3752 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 74506 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14475	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.79	1/1481 (0.1%)	0.88	3/1996 (0.2%)
1	B	0.73	1/1460 (0.1%)	0.85	1/1970 (0.1%)
1	C	0.74	1/1484 (0.1%)	0.86	1/2000 (0.1%)
1	D	0.69	1/1488 (0.1%)	0.86	2/2004 (0.1%)
1	E	0.71	2/1471 (0.1%)	0.87	2/1984 (0.1%)
1	F	0.74	1/1460 (0.1%)	0.90	3/1969 (0.2%)
1	G	0.68	2/1435 (0.1%)	0.88	3/1939 (0.2%)
1	H	0.75	1/1481 (0.1%)	0.89	2/1996 (0.1%)
1	I	0.71	1/1463 (0.1%)	0.86	2/1975 (0.1%)
1	J	0.64	1/1475 (0.1%)	0.85	3/1988 (0.2%)
All	All	0.72	12/14698 (0.1%)	0.87	22/19821 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	150	CYS	CB-SG	8.64	1.97	1.82
1	F	150	CYS	CB-SG	7.76	1.95	1.82
1	D	150	CYS	CB-SG	7.69	1.95	1.82
1	A	150	CYS	CB-SG	7.62	1.95	1.82
1	I	150	CYS	CB-SG	7.42	1.94	1.82
1	G	150	CYS	CB-SG	7.38	1.94	1.82
1	J	150	CYS	CB-SG	7.11	1.94	1.82
1	C	150	CYS	CB-SG	7.10	1.94	1.82
1	E	150	CYS	CB-SG	6.64	1.93	1.82
1	B	150	CYS	CB-SG	6.49	1.93	1.82
1	E	150	CYS	CA-CB	5.35	1.65	1.53
1	G	150	CYS	CA-CB	5.04	1.65	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	150	CYS	CA-CB-SG	9.97	131.94	114.00
1	D	150	CYS	CA-CB-SG	9.86	131.75	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	150	CYS	CA-CB-SG	9.86	131.74	114.00
1	G	150	CYS	CA-CB-SG	9.78	131.60	114.00
1	I	150	CYS	CA-CB-SG	9.56	131.21	114.00
1	B	150	CYS	CA-CB-SG	9.55	131.19	114.00
1	H	150	CYS	CA-CB-SG	9.54	131.18	114.00
1	J	150	CYS	CA-CB-SG	9.24	130.63	114.00
1	C	150	CYS	CA-CB-SG	9.20	130.56	114.00
1	A	150	CYS	CA-CB-SG	9.13	130.43	114.00
1	J	155	GLY	N-CA-C	5.92	127.90	113.10
1	F	73	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	I	50	ASP	C-N-CD	5.59	140.14	128.40
1	E	106	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	G	57	THR	N-CA-C	-5.53	96.07	111.00
1	G	151	MET	CB-CA-C	-5.50	99.41	110.40
1	H	56	ASP	N-CA-C	-5.50	96.16	111.00
1	A	115	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	31	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	4	ILE	CG1-CB-CG2	-5.32	99.70	111.40
1	J	187	LYS	CB-CA-C	-5.26	99.87	110.40
1	A	154	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1458	0	1493	26	0
1	B	1437	0	1454	38	0
1	C	1461	0	1497	25	0
1	D	1465	0	1508	35	0
1	E	1449	0	1479	32	0
1	F	1438	0	1460	32	0
1	G	1415	0	1413	30	0
1	H	1458	0	1493	20	0
1	I	1441	0	1456	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1453	0	1485	34	0
All	All	14475	0	14738	256	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.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:HIS:HD2	1:B:150:CYS:SG	1.53	1.30
1:H:81:HIS:HD2	1:H:150:CYS:SG	1.55	1.29
1:J:81:HIS:HD2	1:J:150:CYS:SG	1.56	1.29
1:G:81:HIS:HD2	1:G:150:CYS:SG	1.56	1.28
1:C:80:HIS:HD2	1:C:150:CYS:SG	1.57	1.27
1:E:119:LEU:HD23	1:E:121:GLU:OE1	1.35	1.26
1:A:81:HIS:HD2	1:A:150:CYS:SG	1.58	1.26
1:J:80:HIS:HD2	1:J:150:CYS:SG	1.62	1.22
1:H:81:HIS:CD2	1:H:150:CYS:SG	2.33	1.21
1:J:81:HIS:CD2	1:J:150:CYS:SG	2.35	1.20
1:A:81:HIS:CD2	1:A:150:CYS:SG	2.36	1.19
1:B:81:HIS:CD2	1:B:150:CYS:SG	2.35	1.18
1:G:81:HIS:CD2	1:G:150:CYS:SG	2.35	1.18
1:J:80:HIS:CD2	1:J:150:CYS:SG	2.44	1.10
1:C:80:HIS:CD2	1:C:150:CYS:SG	2.47	1.08
1:F:187:LYS:O	1:F:188:HIS:CG	2.08	1.07
1:B:103:LEU:HD21	1:D:163:THR:HG21	1.41	1.03
1:J:151:MET:HG2	1:J:156:VAL:HG21	1.42	1.01
1:I:63:HIS:NE2	1:I:100:VAL:HG12	1.79	0.96
1:C:81:HIS:ND1	1:C:150:CYS:SG	2.38	0.95
1:B:101:ALA:HB2	1:B:135:LEU:HD11	1.47	0.95
1:B:79:GLU:OE2	1:B:119:LEU:HD11	1.64	0.95
1:F:81:HIS:ND1	1:F:150:CYS:SG	2.42	0.93
1:E:81:HIS:ND1	1:E:150:CYS:SG	2.41	0.93
1:I:107:ALA:HB3	1:J:156:VAL:HG11	1.52	0.92
1:I:81:HIS:ND1	1:I:150:CYS:SG	2.43	0.91
1:D:81:HIS:ND1	1:D:150:CYS:SG	2.44	0.89
1:D:99:ARG:O	1:D:135:LEU:HD22	1.75	0.87
1:I:63:HIS:CD2	1:I:100:VAL:HG12	2.10	0.85
1:F:187:LYS:O	1:F:188:HIS:CD2	2.29	0.85
1:F:70:LYS:NZ	1:F:188:HIS:HB3	1.95	0.81
1:C:156:VAL:HG21	1:G:107:ALA:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:THR:HG21	1:J:103:LEU:HD21	1.61	0.80
1:E:83:VAL:HG22	1:E:84:PRO:HD2	1.62	0.80
1:B:79:GLU:CD	1:B:119:LEU:HD11	2.02	0.79
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.48	0.78
1:D:99:ARG:O	1:D:135:LEU:CD2	2.35	0.74
1:E:156:VAL:HG21	1:H:104:SER:HB2	1.70	0.74
1:C:54:HIS:HE1	1:C:112:ASP:OD2	1.69	0.74
1:J:151:MET:HG2	1:J:156:VAL:CG2	2.20	0.70
1:D:57:THR:O	1:D:58:ILE:HG13	1.91	0.70
1:E:163:THR:OG1	1:H:103:LEU:HD11	1.91	0.69
1:E:119:LEU:CD2	1:E:121:GLU:OE1	2.28	0.69
1:J:77:MET:HE1	1:J:84:PRO:HG3	1.72	0.69
1:J:80:HIS:HB2	1:J:81:HIS:CD2	2.28	0.67
1:B:155:GLY:CA	1:C:42:GLU:OE2	2.43	0.67
1:C:54:HIS:CE1	1:C:112:ASP:OD2	2.48	0.66
1:F:70:LYS:HZ1	1:F:188:HIS:HB3	1.59	0.66
1:B:119:LEU:HD12	1:B:119:LEU:N	2.10	0.65
1:E:119:LEU:HD23	1:E:121:GLU:CD	2.14	0.65
1:B:83:VAL:HG12	1:B:149:MET:HB2	1.79	0.65
1:B:103:LEU:CD2	1:D:163:THR:HG21	2.23	0.64
1:B:79:GLU:CD	1:B:119:LEU:CD1	2.66	0.64
1:F:83:VAL:HG12	1:F:149:MET:HB2	1.81	0.63
1:D:58:ILE:CG2	1:D:99:ARG:HA	2.28	0.63
1:E:83:VAL:HG22	1:E:84:PRO:CD	2.28	0.63
1:B:83:VAL:CG1	1:B:149:MET:HB2	2.28	0.63
1:I:107:ALA:HB3	1:J:156:VAL:CG1	2.27	0.63
1:B:4:ILE:HD12	1:C:20:VAL:HA	1.81	0.63
1:J:73:ARG:HG3	1:J:73:ARG:HH11	1.64	0.63
1:F:83:VAL:CG1	1:F:149:MET:HB2	2.29	0.62
1:D:42:GLU:OE2	1:G:155:GLY:CA	2.47	0.62
1:J:77:MET:HE2	1:J:84:PRO:HA	1.81	0.61
1:B:119:LEU:HD13	1:B:122:ARG:NH2	2.16	0.61
1:I:65:GLU:OE2	1:J:169:ARG:NH1	2.31	0.61
1:I:107:ALA:CB	1:J:156:VAL:HG11	2.27	0.61
1:H:101:ALA:HB2	1:H:135:LEU:HD11	1.82	0.61
1:F:70:LYS:HZ2	1:F:188:HIS:HB3	1.65	0.61
1:H:4:ILE:HD12	1:J:20:VAL:HA	1.83	0.60
1:G:73:ARG:HG3	1:G:73:ARG:HH11	1.67	0.60
1:A:42:GLU:OE2	1:F:155:GLY:CA	2.50	0.59
1:A:7:GLN:NE2	1:A:34:MET:HE3	2.17	0.59
1:C:156:VAL:HG21	1:G:107:ALA:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:SER:O	1:G:134:LYS:HD2	2.02	0.59
1:E:101:ALA:HB2	1:E:135:LEU:HD11	1.85	0.59
1:J:61:GLU:O	1:J:98:GLY:HA3	2.03	0.58
1:A:73:ARG:HH11	1:A:73:ARG:CG	2.16	0.58
1:B:155:GLY:HA2	1:C:42:GLU:OE2	2.04	0.57
1:D:101:ALA:HB2	1:D:135:LEU:HD11	1.86	0.57
1:B:157:ASN:HD22	1:F:157:ASN:HD22	1.51	0.57
1:J:101:ALA:HB2	1:J:135:LEU:HD11	1.87	0.57
1:B:119:LEU:HD13	1:B:122:ARG:CZ	2.35	0.56
1:D:59:PHE:O	1:D:98:GLY:O	2.23	0.56
1:I:68:LEU:HD11	1:I:186:ILE:HD11	1.88	0.56
1:F:101:ALA:HB2	1:F:135:LEU:HD11	1.86	0.56
1:A:101:ALA:HB2	1:A:135:LEU:HD11	1.87	0.56
1:E:155:GLY:HA3	1:I:42:GLU:OE2	2.06	0.56
1:A:169:ARG:NH1	1:E:65:GLU:OE2	2.39	0.56
1:D:58:ILE:HG21	1:D:99:ARG:HA	1.88	0.56
1:D:60:GLU:HA	1:D:98:GLY:O	2.06	0.56
1:G:154:ARG:O	1:G:157:ASN:CG	2.44	0.55
1:D:57:THR:C	1:D:58:ILE:HG13	2.25	0.55
1:B:61:GLU:O	1:B:98:GLY:HA3	2.07	0.55
1:E:154:ARG:HD2	1:I:39:MET:HG3	1.89	0.55
1:C:61:GLU:HG3	1:C:62:GLN:N	2.21	0.55
1:I:52:SER:CA	1:I:53:VAL:CB	2.85	0.55
1:C:101:ALA:HB2	1:C:135:LEU:HD11	1.88	0.55
1:A:140:VAL:HG12	1:A:169:ARG:HB2	1.90	0.54
1:B:42:GLU:OE2	1:C:155:GLY:HA2	2.08	0.54
1:F:140:VAL:HG12	1:F:169:ARG:HB2	1.89	0.54
1:H:140:VAL:HG12	1:H:169:ARG:HB2	1.90	0.54
1:H:56:ASP:HB3	1:H:105:LYS:HD3	1.90	0.54
1:G:99:ARG:HH11	1:G:99:ARG:HA	1.73	0.53
1:E:60:GLU:O	1:E:61:GLU:C	2.46	0.53
1:B:103:LEU:HB3	1:D:151:MET:SD	2.48	0.53
1:C:61:GLU:O	1:C:98:GLY:HA3	2.08	0.53
1:G:101:ALA:HB2	1:G:135:LEU:HD11	1.90	0.53
1:D:140:VAL:HG12	1:D:169:ARG:HB2	1.89	0.53
1:B:119:LEU:CD1	1:B:119:LEU:N	2.72	0.53
1:A:125:THR:HG21	1:E:63:HIS:CD2	2.44	0.52
1:I:101:ALA:HB2	1:I:135:LEU:HD11	1.89	0.52
1:I:63:HIS:NE2	1:I:95:PRO:HG2	2.25	0.52
1:B:140:VAL:HG12	1:B:169:ARG:HB2	1.92	0.52
1:J:76:SER:O	1:J:77:MET:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:GLU:O	1:J:98:GLY:CA	2.58	0.52
1:B:157:ASN:ND2	1:F:157:ASN:HD22	2.07	0.52
1:I:140:VAL:HG12	1:I:169:ARG:HB2	1.92	0.52
1:C:80:HIS:HB2	1:C:81:HIS:ND1	2.25	0.51
1:B:93:TYR:CE2	1:B:135:LEU:HD21	2.44	0.51
1:I:22:GLU:HG3	1:I:29:LEU:CD1	2.40	0.51
1:F:125:THR:O	1:F:129:GLU:HG2	2.10	0.51
1:E:140:VAL:HG12	1:E:169:ARG:HB2	1.91	0.51
1:H:151:MET:HE1	1:H:161:THR:HG21	1.92	0.51
1:I:63:HIS:CE1	1:I:100:VAL:HG12	2.42	0.51
1:I:63:HIS:NE2	1:I:95:PRO:CG	2.74	0.51
1:A:22:GLU:HG3	1:A:29:LEU:CD1	2.41	0.51
1:A:125:THR:HG21	1:E:63:HIS:HD2	1.77	0.50
1:F:61:GLU:O	1:F:98:GLY:HA3	2.11	0.50
1:F:96:GLN:NE2	1:F:138:LEU:CD2	2.75	0.50
1:E:22:GLU:CG	1:E:29:LEU:CD1	2.90	0.50
1:B:22:GLU:HG3	1:B:29:LEU:CD1	2.41	0.50
1:D:151:MET:HE1	1:D:161:THR:HG21	1.93	0.50
1:C:61:GLU:HG3	1:C:62:GLN:H	1.75	0.50
1:G:58:ILE:HA	1:G:100:VAL:O	2.11	0.50
1:C:140:VAL:HG12	1:C:169:ARG:HB2	1.93	0.50
1:E:22:GLU:HG3	1:E:29:LEU:CD1	2.42	0.50
1:H:151:MET:CE	1:H:161:THR:HG21	2.42	0.49
1:E:125:THR:O	1:E:129:GLU:HG2	2.11	0.49
1:A:73:ARG:NH1	1:A:73:ARG:CG	2.73	0.49
1:A:125:THR:O	1:A:129:GLU:HG2	2.11	0.49
1:I:22:GLU:CG	1:I:29:LEU:CD1	2.90	0.49
1:G:125:THR:O	1:G:129:GLU:HG2	2.12	0.49
1:I:125:THR:O	1:I:129:GLU:HG2	2.11	0.49
1:D:125:THR:O	1:D:129:GLU:HG2	2.13	0.49
1:A:103:LEU:HD23	1:B:151:MET:HG3	1.93	0.49
1:H:125:THR:O	1:H:129:GLU:HG2	2.13	0.49
1:B:125:THR:O	1:B:129:GLU:HG2	2.12	0.49
1:H:22:GLU:CG	1:H:29:LEU:CD1	2.90	0.49
1:E:119:LEU:CD2	1:E:121:GLU:CD	2.80	0.49
1:B:22:GLU:CG	1:B:29:LEU:CD1	2.91	0.49
1:H:22:GLU:HG3	1:H:29:LEU:CD1	2.42	0.49
1:C:125:THR:O	1:C:129:GLU:HG2	2.13	0.48
1:I:22:GLU:CG	1:I:29:LEU:HD11	2.43	0.48
1:E:22:GLU:CG	1:E:29:LEU:HD11	2.44	0.48
1:F:22:GLU:HG3	1:F:29:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:22:GLU:CG	1:J:29:LEU:CD1	2.91	0.48
1:A:22:GLU:CG	1:A:29:LEU:CD1	2.90	0.48
1:F:103:LEU:HB3	1:I:151:MET:CE	2.43	0.48
1:A:42:GLU:OE2	1:F:155:GLY:HA2	2.14	0.48
1:H:22:GLU:CG	1:H:29:LEU:HD11	2.44	0.48
1:J:22:GLU:HG3	1:J:29:LEU:CD1	2.43	0.48
1:H:155:GLY:CA	1:J:42:GLU:OE2	2.60	0.48
1:B:55:PHE:HZ	1:B:106:LEU:HD12	1.79	0.48
1:D:22:GLU:HG3	1:D:29:LEU:CD1	2.44	0.48
1:G:22:GLU:HG3	1:G:29:LEU:CD1	2.44	0.48
1:A:22:GLU:CG	1:A:29:LEU:HD11	2.44	0.48
1:B:22:GLU:CG	1:B:29:LEU:HD11	2.44	0.47
1:D:22:GLU:CG	1:D:29:LEU:CD1	2.92	0.47
1:G:73:ARG:HG3	1:G:73:ARG:NH1	2.28	0.47
1:F:22:GLU:CG	1:F:29:LEU:CD1	2.93	0.47
1:F:149:MET:C	1:F:151:MET:N	2.68	0.47
1:I:52:SER:HA	1:I:53:VAL:CB	2.44	0.47
1:G:22:GLU:CG	1:G:29:LEU:CD1	2.92	0.47
1:C:80:HIS:HB2	1:C:81:HIS:CE1	2.50	0.46
1:D:151:MET:HB3	1:D:151:MET:HE3	1.57	0.46
1:J:22:GLU:CG	1:J:29:LEU:HD11	2.45	0.46
1:A:122:ARG:NE	1:E:60:GLU:OE2	2.41	0.46
1:G:22:GLU:CG	1:G:29:LEU:HD11	2.46	0.46
1:C:154:ARG:O	1:C:157:ASN:CG	2.54	0.46
1:B:187:LYS:O	1:B:188:HIS:C	2.54	0.46
1:B:73:ARG:NH2	1:G:73:ARG:HH22	2.14	0.46
1:B:61:GLU:O	1:B:98:GLY:CA	2.64	0.46
1:G:61:GLU:O	1:G:62:GLN:CB	2.64	0.46
1:H:121:GLU:CD	1:H:121:GLU:H	2.18	0.46
1:F:177:LYS:HE2	1:I:176:ASP:OD2	2.14	0.46
1:D:149:MET:C	1:D:151:MET:N	2.69	0.45
1:F:96:GLN:NE2	1:F:138:LEU:HD21	2.31	0.45
1:C:103:LEU:HB3	1:F:151:MET:CE	2.45	0.45
1:D:22:GLU:CG	1:D:29:LEU:HD11	2.46	0.45
1:G:149:MET:C	1:G:151:MET:N	2.70	0.45
1:G:187:LYS:O	1:G:188:HIS:CB	2.64	0.45
1:H:119:LEU:HB3	1:H:121:GLU:OE1	2.16	0.45
1:A:60:GLU:OE1	1:B:80:HIS:HE1	2.00	0.45
1:C:187:LYS:O	1:C:188:HIS:C	2.55	0.45
1:D:27:GLU:OE2	1:J:60:GLU:O	2.34	0.45
1:F:4:ILE:HD11	1:F:41:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:HIS:O	1:E:56:ASP:N	2.49	0.45
1:D:42:GLU:OE2	1:G:155:GLY:HA2	2.17	0.45
1:A:60:GLU:OE1	1:B:80:HIS:CE1	2.70	0.45
1:C:73:ARG:O	1:F:158:LYS:HE3	2.17	0.45
1:F:22:GLU:CG	1:F:29:LEU:HD11	2.47	0.44
1:G:61:GLU:O	1:G:62:GLN:HB2	2.17	0.44
1:D:159:PRO:HG2	1:G:73:ARG:NH1	2.32	0.44
1:J:73:ARG:NH1	1:J:73:ARG:HG3	2.30	0.44
1:F:61:GLU:HG3	1:F:62:GLN:N	2.31	0.44
1:D:55:PHE:C	1:D:57:THR:H	2.20	0.44
1:D:151:MET:CE	1:D:161:THR:HB	2.47	0.44
1:J:77:MET:CE	1:J:84:PRO:HG3	2.45	0.43
1:I:149:MET:C	1:I:151:MET:N	2.71	0.43
1:A:149:MET:C	1:A:151:MET:N	2.70	0.43
1:F:96:GLN:HE21	1:F:138:LEU:HD21	1.84	0.43
1:I:63:HIS:CE1	1:J:121:GLU:HG2	2.54	0.43
1:D:58:ILE:HG21	1:D:99:ARG:HG2	2.00	0.43
1:G:120:GLN:OE1	1:G:163:THR:OG1	2.37	0.43
1:F:151:MET:HG3	1:F:151:MET:O	2.19	0.42
1:D:172:PHE:CE1	1:D:178:LEU:HG	2.54	0.42
1:E:154:ARG:HG3	1:I:39:MET:HG3	2.02	0.42
1:D:55:PHE:C	1:D:57:THR:N	2.73	0.42
1:A:131:MET:O	1:A:135:LEU:HB2	2.20	0.42
1:A:129:GLU:CD	1:A:169:ARG:HH21	2.20	0.42
1:D:58:ILE:HG21	1:D:99:ARG:CA	2.49	0.42
1:B:149:MET:C	1:B:151:MET:N	2.73	0.42
1:F:78:CYS:SG	1:F:81:HIS:HB2	2.60	0.42
1:H:172:PHE:CE1	1:H:178:LEU:HG	2.55	0.42
1:H:149:MET:C	1:H:151:MET:N	2.74	0.42
1:E:4:ILE:HD11	1:E:41:GLU:HB2	2.02	0.42
1:D:58:ILE:HG22	1:D:99:ARG:HA	2.00	0.42
1:E:149:MET:C	1:E:151:MET:N	2.72	0.42
1:J:77:MET:HE2	1:J:84:PRO:CA	2.49	0.41
1:E:169:ARG:NH1	1:H:65:GLU:OE2	2.31	0.41
1:E:59:PHE:CE1	1:E:99:ARG:HG2	2.56	0.41
1:G:158:LYS:NZ	1:J:107:ALA:HB1	2.35	0.41
1:I:78:CYS:SG	1:I:81:HIS:HB2	2.61	0.41
1:E:78:CYS:SG	1:E:81:HIS:HB2	2.60	0.41
1:E:59:PHE:HE1	1:E:99:ARG:HG2	1.86	0.41
1:C:168:VAL:HG22	1:G:65:GLU:OE1	2.20	0.41
1:G:4:ILE:HD11	1:G:41:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:PHE:CE1	1:E:178:LEU:HG	2.56	0.41
1:J:54:HIS:O	1:J:105:LYS:HG3	2.20	0.41
1:J:80:HIS:HD2	1:J:81:HIS:HD2	1.68	0.41
1:J:151:MET:O	1:J:156:VAL:HG23	2.21	0.41
1:I:65:GLU:OE1	1:J:168:VAL:HG22	2.20	0.41
1:G:187:LYS:O	1:G:188:HIS:HB2	2.21	0.41
1:D:136:LYS:N	1:D:137:PRO:HD3	2.36	0.41
1:I:187:LYS:O	1:I:188:HIS:C	2.59	0.41
1:B:118:GLN:C	1:B:119:LEU:HD12	2.41	0.41
1:D:78:CYS:SG	1:D:81:HIS:HB2	2.61	0.41
1:B:107:ALA:HB3	1:D:156:VAL:HG21	2.03	0.41
1:A:32:THR:N	1:A:33:PRO:CD	2.84	0.40
1:F:136:LYS:N	1:F:137:PRO:HD3	2.37	0.40
1:I:63:HIS:CD2	1:I:63:HIS:O	2.74	0.40
1:E:136:LYS:N	1:E:137:PRO:HD3	2.37	0.40
1:I:172:PHE:CE1	1:I:178:LEU:HG	2.56	0.40
1:G:172:PHE:CE1	1:G:178:LEU:HG	2.57	0.40
1:A:172:PHE:CE1	1:A:178:LEU:HG	2.57	0.40
1:C:149:MET:C	1:C:151:MET:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/202 (91%)	181 (98%)	2 (1%)	1 (0%)	34	48
1	B	184/202 (91%)	180 (98%)	3 (2%)	1 (0%)	34	48
1	C	184/202 (91%)	180 (98%)	3 (2%)	1 (0%)	34	48
1	D	184/202 (91%)	175 (95%)	8 (4%)	1 (0%)	34	48
1	E	184/202 (91%)	179 (97%)	4 (2%)	1 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	184/202 (91%)	181 (98%)	2 (1%)	1 (0%)	34 48
1	G	184/202 (91%)	181 (98%)	2 (1%)	1 (0%)	34 48
1	H	184/202 (91%)	181 (98%)	2 (1%)	1 (0%)	34 48
1	I	184/202 (91%)	176 (96%)	4 (2%)	4 (2%)	8 9
1	J	184/202 (91%)	182 (99%)	1 (0%)	1 (0%)	34 48
All	All	1840/2020 (91%)	1796 (98%)	31 (2%)	13 (1%)	26 38

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	53	VAL
1	E	150	CYS
1	F	150	CYS
1	I	52	SER
1	I	54	HIS
1	A	150	CYS
1	B	150	CYS
1	D	150	CYS
1	G	150	CYS
1	H	150	CYS
1	I	150	CYS
1	J	150	CYS
1	C	150	CYS

5.3.2 Protein sidechains (i)

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	160/177 (90%)	154 (96%)	6 (4%)	40 60
1	B	154/177 (87%)	151 (98%)	3 (2%)	65 83
1	C	161/177 (91%)	153 (95%)	8 (5%)	30 48
1	D	162/177 (92%)	158 (98%)	4 (2%)	55 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	158/177 (89%)	149 (94%)	9 (6%)	25 40
1	F	155/177 (88%)	149 (96%)	6 (4%)	39 59
1	G	149/177 (84%)	141 (95%)	8 (5%)	27 43
1	H	160/177 (90%)	155 (97%)	5 (3%)	47 69
1	I	155/177 (88%)	148 (96%)	7 (4%)	34 52
1	J	159/177 (90%)	151 (95%)	8 (5%)	30 48
All	All	1573/1770 (89%)	1509 (96%)	64 (4%)	37 57

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	PRO
1	A	27	GLU
1	A	115	ARG
1	A	136	LYS
1	A	150	CYS
1	A	180	SER
1	B	135	LEU
1	B	150	CYS
1	B	180	SER
1	C	57	THR
1	C	60	GLU
1	C	62	GLN
1	C	80	HIS
1	C	106	LEU
1	C	150	CYS
1	C	156	VAL
1	C	180	SER
1	D	4	ILE
1	D	96	GLN
1	D	150	CYS
1	D	180	SER
1	E	3	GLN
1	E	34	MET
1	E	55	PHE
1	E	83	VAL
1	E	106	LEU
1	E	115	ARG
1	E	119	LEU
1	E	150	CYS

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Mol	Chain	Res	Type
1	E	180	SER
1	F	34	MET
1	F	97	ASN
1	F	150	CYS
1	F	154	ARG
1	F	177	LYS
1	F	180	SER
1	G	34	MET
1	G	99	ARG
1	G	106	LEU
1	G	134	LYS
1	G	136	LYS
1	G	150	CYS
1	G	177	LYS
1	G	180	SER
1	H	18	GLU
1	H	49	LYS
1	H	55	PHE
1	H	150	CYS
1	H	180	SER
1	I	55	PHE
1	I	64	GLU
1	I	99	ARG
1	I	106	LEU
1	I	150	CYS
1	I	177	LYS
1	I	180	SER
1	J	80	HIS
1	J	105	LYS
1	J	115	ARG
1	J	150	CYS
1	J	154	ARG
1	J	156	VAL
1	J	177	LYS
1	J	180	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	81	HIS
1	A	188	HIS

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Mol	Chain	Res	Type
1	B	80	HIS
1	B	81	HIS
1	B	96	GLN
1	B	157	ASN
1	C	54	HIS
1	C	80	HIS
1	C	97	ASN
1	E	63	HIS
1	E	97	ASN
1	F	96	GLN
1	F	97	ASN
1	F	188	HIS
1	G	63	HIS
1	G	81	HIS
1	H	81	HIS
1	H	97	ASN
1	I	148	HIS
1	J	80	HIS
1	J	81	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	186/202 (92%)	-0.11	4 (2%)	65	64	25, 39, 72, 98	0
1	B	186/202 (92%)	-0.03	8 (4%)	39	40	26, 43, 79, 102	0
1	C	186/202 (92%)	-0.03	4 (2%)	65	64	26, 42, 75, 96	0
1	D	186/202 (92%)	0.18	14 (7%)	17	17	26, 44, 93, 123	0
1	E	186/202 (92%)	-0.01	8 (4%)	39	40	28, 46, 81, 107	0
1	F	186/202 (92%)	0.07	14 (7%)	17	17	28, 43, 88, 112	0
1	G	186/202 (92%)	0.22	13 (6%)	19	19	27, 48, 90, 116	0
1	H	186/202 (92%)	-0.20	3 (1%)	74	74	28, 41, 68, 97	0
1	I	186/202 (92%)	0.26	9 (4%)	34	35	28, 49, 88, 103	0
1	J	186/202 (92%)	0.50	22 (11%)	6	6	32, 51, 93, 116	0
All	All	1860/2020 (92%)	0.08	99 (5%)	30	30	25, 45, 85, 123	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	52	SER	7.3
1	D	59	PHE	7.0
1	J	56	ASP	6.8
1	D	57	THR	6.6
1	J	53	VAL	6.1
1	G	54	HIS	5.5
1	F	59	PHE	5.4
1	I	53	VAL	5.3
1	E	3	GLN	5.0
1	J	58	ILE	4.9
1	G	51	PRO	4.7
1	G	55	PHE	4.7
1	E	156	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	3	GLN	4.4
1	I	51	PRO	4.4
1	J	48	LYS	4.3
1	D	58	ILE	4.2
1	D	3	GLN	4.2
1	I	54	HIS	4.2
1	J	50	ASP	4.2
1	F	49	LYS	4.0
1	B	155	GLY	3.9
1	F	56	ASP	3.8
1	G	50	ASP	3.7
1	G	53	VAL	3.7
1	J	54	HIS	3.7
1	F	150	CYS	3.5
1	D	52	SER	3.5
1	J	136	LYS	3.5
1	J	174	ASN	3.5
1	D	157	ASN	3.4
1	H	174	ASN	3.4
1	J	25	ASP	3.4
1	G	52	SER	3.3
1	G	174	ASN	3.3
1	A	174	ASN	3.3
1	D	53	VAL	3.3
1	D	56	ASP	3.2
1	F	60	GLU	3.2
1	C	174	ASN	3.1
1	B	3	GLN	3.1
1	J	99	ARG	3.1
1	B	4	ILE	3.1
1	B	48	LYS	3.1
1	E	27	GLU	3.0
1	G	49	LYS	3.0
1	J	97	ASN	3.0
1	J	49	LYS	3.0
1	F	57	THR	2.9
1	J	98	GLY	2.9
1	J	57	THR	2.9
1	G	48	LYS	2.8
1	J	27	GLU	2.8
1	H	3	GLN	2.8
1	I	3	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	4	ILE	2.7
1	F	99	ARG	2.7
1	B	57	THR	2.7
1	F	54	HIS	2.7
1	F	53	VAL	2.6
1	B	56	ASP	2.6
1	J	4	ILE	2.6
1	D	60	GLU	2.6
1	D	98	GLY	2.6
1	F	98	GLY	2.6
1	I	138	LEU	2.6
1	D	155	GLY	2.5
1	J	60	GLU	2.5
1	I	150	CYS	2.5
1	C	62	GLN	2.5
1	G	57	THR	2.5
1	E	54	HIS	2.5
1	A	155	GLY	2.5
1	B	150	CYS	2.4
1	A	3	GLN	2.3
1	E	50	ASP	2.3
1	E	49	LYS	2.3
1	G	133	GLU	2.2
1	J	62	GLN	2.2
1	D	4	ILE	2.2
1	F	188	HIS	2.2
1	J	30	ILE	2.2
1	F	50	ASP	2.1
1	B	133	GLU	2.1
1	F	155	GLY	2.1
1	C	155	GLY	2.1
1	D	150	CYS	2.1
1	F	58	ILE	2.1
1	I	56	ASP	2.1
1	I	50	ASP	2.1
1	J	188	HIS	2.1
1	E	157	ASN	2.1
1	C	98	GLY	2.1
1	A	48	LYS	2.1
1	G	45	ALA	2.1
1	G	155	GLY	2.0
1	D	48	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	52	SER	2.0
1	E	55	PHE	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.