



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:11 AM GMT

PDB ID : 3HJH
Title : A rigid N-terminal clamp restrains the motor domains of the bacterial transcription-repair coupling factor
Authors : Murphy, M.; Gong, P.; Ralto, K.; Manelyte, L.; Savery, N.; Theis, K.
Deposited on : 2009-05-21
Resolution : 1.95 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

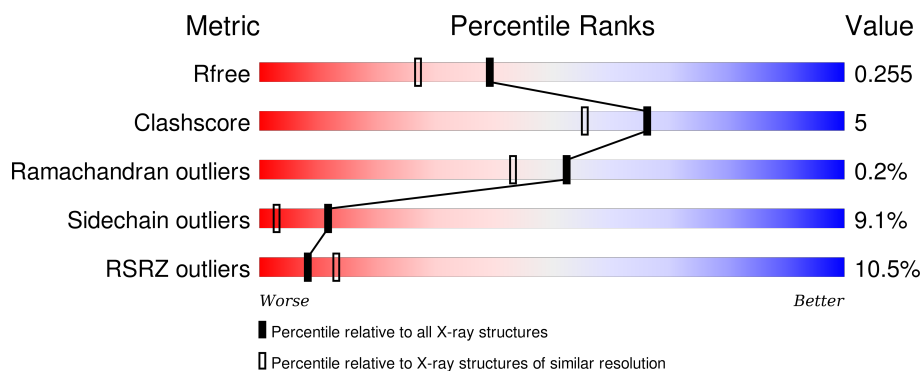
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 $\leq 5\%$. 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	483	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3888 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 Transcription-repair-coupling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3569	2270	622	663	14			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	LYS	-	EXPRESSION TAG	UNP P30958
A	472	LEU	-	EXPRESSION TAG	UNP P30958
A	473	ALA	-	EXPRESSION TAG	UNP P30958
A	474	ALA	-	EXPRESSION TAG	UNP P30958
A	475	ALA	-	EXPRESSION TAG	UNP P30958
A	476	LEU	-	EXPRESSION TAG	UNP P30958
A	477	GLU	-	EXPRESSION TAG	UNP P30958
A	478	HIS	-	EXPRESSION TAG	UNP P30958
A	479	HIS	-	EXPRESSION TAG	UNP P30958
A	480	HIS	-	EXPRESSION TAG	UNP P30958
A	481	HIS	-	EXPRESSION TAG	UNP P30958
A	482	HIS	-	EXPRESSION TAG	UNP P30958
A	483	HIS	-	EXPRESSION TAG	UNP P30958

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		

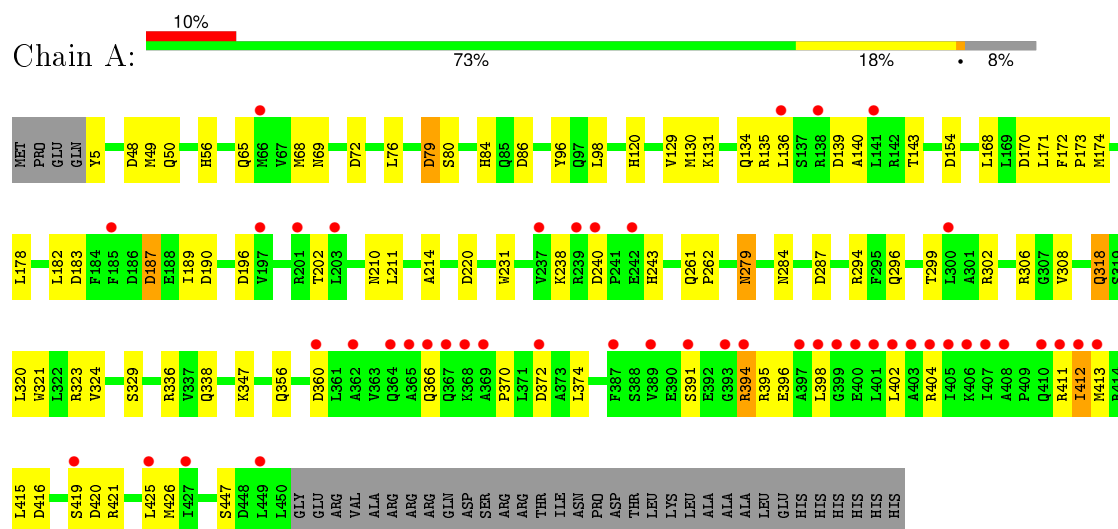
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	318	Total	O	0	0
			318	318		

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 ($\text{RSRZ} > 2$). 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: Transcription-repair-coupling factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.06 Å 157.65 Å 35.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.03 – 1.95 42.03 – 1.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.03-1.95) 99.5 (42.03-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.92 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.210 , 0.257 0.213 , 0.255	Depositor DCC
R_{free} test set	1788 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 36838 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3888	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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

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	0.47	0/3652	0.79	16/4961 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	287	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	170	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	220	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	48	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	420	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	79	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	196	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	187	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	139	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	72	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	360	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	240	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	372	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	190	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	154	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3569	0	3536	35	0
2	A	1	0	0	0	0
3	A	318	0	0	11	0
All	All	3888	0	3536	35	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 5.

All (35) 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:140:ALA:O	3:A:777:HOH:O	2.02	0.77
1:A:135:ARG:O	3:A:776:HOH:O	2.11	0.68
1:A:143:THR:HB	3:A:777:HOH:O	1.95	0.67
1:A:84:HIS:HD2	1:A:86:ASP:H	1.46	0.62
1:A:5:TYR:N	3:A:784:HOH:O	2.32	0.62
1:A:284:ASN:HD21	1:A:338:GLN:HG2	1.63	0.62
1:A:320:LEU:HD23	3:A:619:HOH:O	2.04	0.57
1:A:279:ASN:H	1:A:279:ASN:HD22	1.53	0.57
1:A:318:GLN:HE21	1:A:318:GLN:H	1.54	0.55
1:A:130:MET:HA	1:A:134:GLN:HE22	1.72	0.55
1:A:168:LEU:CD2	1:A:183:ASP:HB3	2.37	0.53
1:A:284:ASN:ND2	1:A:336:ARG:HH11	2.09	0.50
1:A:296:GLN:HE22	1:A:324:VAL:H	1.59	0.50
1:A:56:HIS:HB2	1:A:69:ASN:HD21	1.78	0.48
1:A:231:TRP:CZ2	1:A:243:HIS:HE1	2.32	0.48
1:A:131:LYS:NZ	3:A:565:HOH:O	2.46	0.47
1:A:96:TYR:O	1:A:120:HIS:HE1	1.97	0.47
1:A:302:ARG:NH2	1:A:306:ARG:HE	2.13	0.46
1:A:173:PRO:HG3	1:A:211:LEU:HD22	1.98	0.46
1:A:299:THR:HG21	1:A:321:TRP:CE3	2.52	0.45
1:A:76:LEU:O	1:A:79:ASP:HB2	2.16	0.45
1:A:279:ASN:N	1:A:279:ASN:HD22	2.16	0.43
1:A:120:HIS:HD2	3:A:529:HOH:O	2.00	0.43
1:A:174:MET:HG3	1:A:214:ALA:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:H	1:A:412:ILE:HD13	1.84	0.42
1:A:136:LEU:HD23	1:A:189:ILE:HD11	2.01	0.42
1:A:238:LYS:H	1:A:243:HIS:CD2	2.36	0.42
1:A:261:GLN:N	1:A:262:PRO:CD	2.82	0.42
1:A:129:VAL:HB	3:A:800:HOH:O	2.19	0.42
1:A:84:HIS:CD2	1:A:86:ASP:HB2	2.55	0.41
1:A:68:MET:HE3	1:A:68:MET:HB2	1.83	0.41
1:A:394:ARG:C	3:A:678:HOH:O	2.59	0.41
1:A:394:ARG:C	1:A:396:GLU:H	2.23	0.41
1:A:323:ARG:CZ	3:A:577:HOH:O	2.67	0.40
1:A:210:ASN:ND2	3:A:706:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	444/483 (92%)	431 (97%)	12 (3%)	1 (0%)	52 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	386/418 (92%)	351 (91%)	35 (9%)	12 3

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MET
1	A	50	GLN
1	A	65	GLN
1	A	80	SER
1	A	98	LEU
1	A	171	LEU
1	A	172	PHE
1	A	178	LEU
1	A	182	LEU
1	A	187	ASP
1	A	202	THR
1	A	279	ASN
1	A	294	ARG
1	A	308	VAL
1	A	318	GLN
1	A	329	SER
1	A	347	LYS
1	A	356	GLN
1	A	366	GLN
1	A	374	LEU
1	A	391	SER
1	A	394	ARG
1	A	395	ARG
1	A	398	LEU
1	A	402	LEU
1	A	404	ARG
1	A	411	ARG
1	A	412	ILE
1	A	413	MET
1	A	415	LEU
1	A	419	SER
1	A	421	ARG
1	A	425	LEU
1	A	426	MET
1	A	447	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	84	HIS
1	A	97	GLN
1	A	115	GLN
1	A	120	HIS
1	A	126	HIS
1	A	134	GLN
1	A	243	HIS
1	A	246	GLN
1	A	279	ASN
1	A	284	ASN
1	A	296	GLN
1	A	318	GLN
1	A	366	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	446/483 (92%)	0.79	47 (10%) 8 13	3, 13, 29, 45	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	ALA	10.5
1	A	398	LEU	9.1
1	A	136	LEU	8.9
1	A	403	ALA	7.1
1	A	367	GLN	6.9
1	A	397	ALA	6.6
1	A	366	GLN	6.5
1	A	402	LEU	5.9
1	A	239	ARG	4.7
1	A	411	ARG	4.7
1	A	401	LEU	4.6
1	A	369	ALA	4.5
1	A	400	GLU	4.4
1	A	364	GLN	4.1
1	A	410	GLN	4.1
1	A	393	GLY	3.9
1	A	362	ALA	3.8
1	A	240	ASP	3.6
1	A	203	LEU	3.6
1	A	427	ILE	3.5
1	A	394	ARG	3.3
1	A	399	GLY	3.1
1	A	407	ILE	3.1
1	A	406	LYS	3.0
1	A	360	ASP	3.0
1	A	404	ARG	2.9
1	A	413	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	368	LYS	2.9
1	A	185	PHE	2.8
1	A	66	MET	2.7
1	A	449	LEU	2.7
1	A	391	SER	2.7
1	A	372	ASP	2.6
1	A	300	LEU	2.6
1	A	405	ILE	2.5
1	A	197	VAL	2.5
1	A	389	VAL	2.5
1	A	201	ARG	2.4
1	A	419	SER	2.4
1	A	242	GLU	2.4
1	A	408	ALA	2.4
1	A	141	LEU	2.3
1	A	237	VAL	2.3
1	A	412	ILE	2.2
1	A	387	PHE	2.1
1	A	425	LEU	2.1
1	A	138	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	CO	A	484	1/1	0.99	0.07	-	26,26,26,26	1

6.5 Other polymers

There are no such residues in this entry.