wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 11:39 PM EDT

PDB ID	:	2QM4
Title	:	Crystal structure of human XLF/Cernunnos, a non-homologous end-joining factor
Authors	:	Li, Y.; Chirgadze, D.Y.; Sibanda, B.L.; Bolanos-Garcia, V.M.; Davies, O.R.; Blundell, T.L.
Deposited on	:	2007-07-14
Resolution	:	2.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

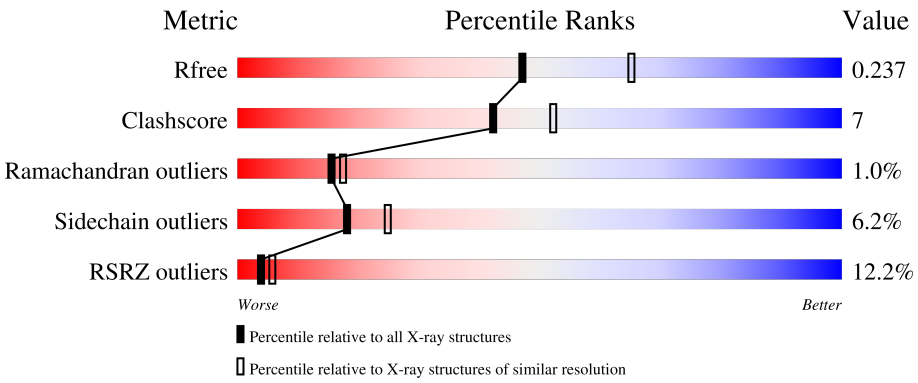
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of 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 <=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	235	9% 81% 15%
1	B	235	10% 79% 15%
1	C	235	13% 76% 19%
1	D	235	14% 77% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7510 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 Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	232	1864	1191	312	344	6	11	0	7	0
1	B	225	1821	1167	304	334	6	10	0	10	0
1	C	229	1818	1160	305	337	6	10	0	4	0
1	D	225	1775	1137	292	330	6	10	0	7	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
A	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
B	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
C	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
D	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4

- Molecule 2 is water.

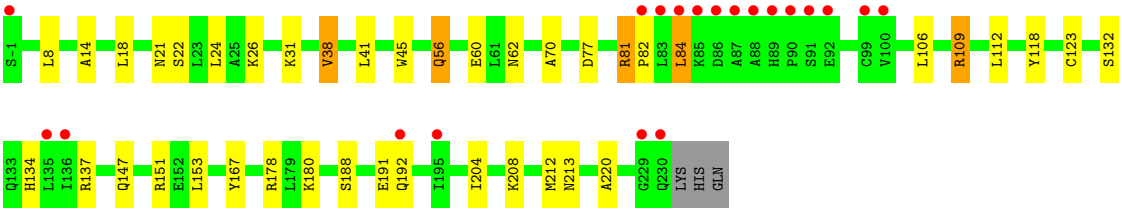
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	73	73	73	0	0
			Total	O		
2	B	49	49	49	0	0
			Total	O		
2	C	47	47	47	0	0
			Total	O		
2	D	63	63	63	0	0

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.

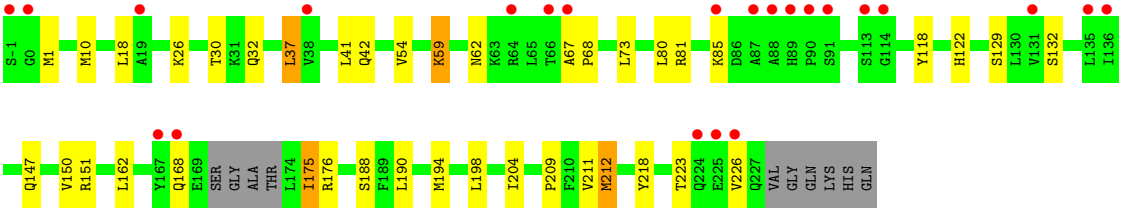
• Molecule 1: Non-homologous end-joining factor 1

Chain A:



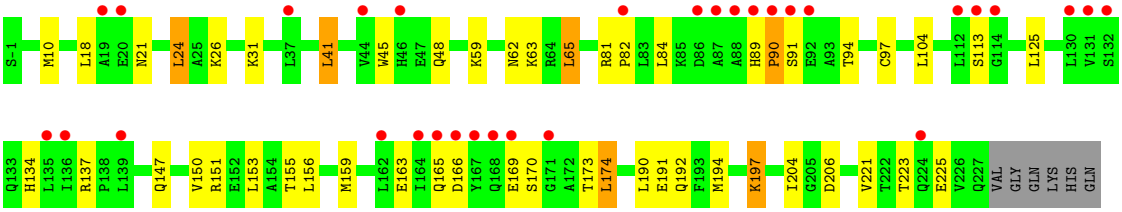
• Molecule 1: Non-homologous end-joining factor 1

Chain B:



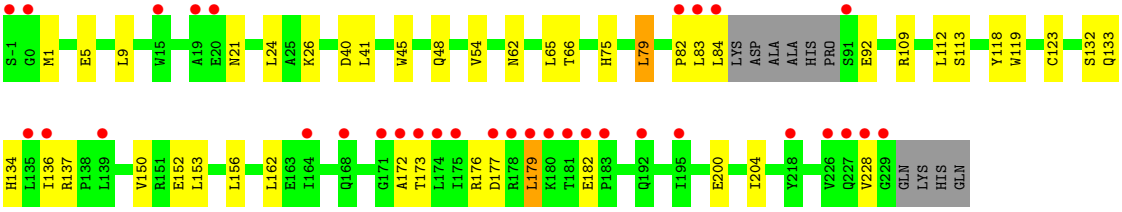
• Molecule 1: Non-homologous end-joining factor 1

Chain C:



• Molecule 1: Non-homologous end-joining factor 1

Chain D:


S-1
G0
M1
E5
L9
W15
A19
E20
N21
L24
A25
K26
D40
L41
W45
Q48
V54
N62
L65
T66
H75
L79
P82
L83
L84
LYS
ASP
ALA
ALA
HIS
PRO
S91
E92
R109
L112
S113
Y118
W119
C123
S132
Q133
H134
L135
I136
R137
P138
L139
V150
R151
E152
L153
L156
L162
E163
I164
Q168
G171
A172
T173
L174
I175
R176
D177
R178
L179
K180
T181
E182
P183
Q192
I195
E200
I204
Y218
V226
Q227
V228
G229
GLN
LYS
HIS
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.74Å 92.91Å 103.69Å 90.00° 106.22° 90.00°	Depositor
Resolution (Å)	37.01 – 2.30 37.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.01-2.30) 92.8 (37.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	6.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.239 0.180 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7510	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.62	0/1909	0.69	0/2570
1	B	0.60	0/1875	0.65	1/2526 (0.0%)
1	C	0.61	2/1856 (0.1%)	0.69	3/2500 (0.1%)
1	D	0.66	0/1821	0.73	0/2454
All	All	0.62	2/7461 (0.0%)	0.69	4/10050 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	GLU	CD-OE1	6.90	1.33	1.25
1	C	163	GLU	CD-OE2	6.39	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	PRO	N-CA-CB	6.40	110.98	103.30
1	B	37	LEU	CA-CB-CG	5.52	127.99	115.30
1	C	174	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	65	LEU	CA-CB-CG	5.09	127.01	115.30

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	1864	0	1886	36	0
1	B	1821	0	1825	28	0
1	C	1818	0	1821	20	0
1	D	1775	0	1765	31	0
2	A	73	0	0	1	0
2	B	49	0	0	2	0
2	C	47	0	0	1	0
2	D	63	0	0	3	0
All	All	7510	0	7297	100	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 7.

The worst 5 of 100 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:109:ARG:HH11	1:A:109:ARG:HG3	1.24	1.00
1:A:62:ASN:HD21	1:A:118:TYR:H	1.20	0.89
1:A:208:LYS:NZ	1:A:212[A]:MSE:HE3	1.87	0.89
1:B:211:VAL:HG12	1:B:212[A]:MSE:HE3	1.55	0.87
1:D:62:ASN:HD21	1:D:118:TYR:H	1.28	0.82

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	237/235 (101%)	228 (96%)	9 (4%)	0	100	100
1	B	231/235 (98%)	219 (95%)	12 (5%)	0	100	100
1	C	231/235 (98%)	218 (94%)	8 (4%)	5 (2%)	6	5
1	D	228/235 (97%)	214 (94%)	10 (4%)	4 (2%)	8	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	927/940 (99%)	879 (95%)	39 (4%)	9 (1%)	15 17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	HIS
1	C	90	PRO
1	C	91	SER
1	D	92	GLU
1	D	172	ALA

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	208/198 (105%)	198 (95%)	10 (5%)	25 36
1	B	201/198 (102%)	187 (93%)	14 (7%)	15 19
1	C	200/198 (101%)	181 (90%)	19 (10%)	8 10
1	D	195/198 (98%)	185 (95%)	10 (5%)	24 33
All	All	804/792 (102%)	751 (93%)	53 (7%)	18 22

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	GLN
1	C	125	LEU
1	D	177	ASP
1	C	59	LYS
1	C	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	75	HIS
1	D	165	GLN
1	C	32	GLN
1	C	122	HIS
1	C	134	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	223/235 (94%)	0.66	20 (8%)	9	12	41, 54, 85, 112	2 (0%)
1	B	216/235 (91%)	0.77	23 (10%)	6	8	44, 57, 89, 106	1 (0%)
1	C	220/235 (93%)	1.01	31 (14%)	2	3	30, 58, 83, 94	3 (1%)
1	D	216/235 (91%)	0.88	33 (15%)	2	3	40, 53, 74, 96	0
All	All	875/940 (93%)	0.83	107 (12%)	4	6	30, 55, 85, 112	6 (0%)

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	ALA	9.9
1	B	88	ALA	7.7
1	C	20	GLU	6.4
1	B	90	PRO	6.4
1	C	113	SER	6.4

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.