

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 3W03

Title : XLF-XRCC4 complex

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Deposited on : 2012-10-17

Resolution : 8.49 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 (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS: 2.36

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)

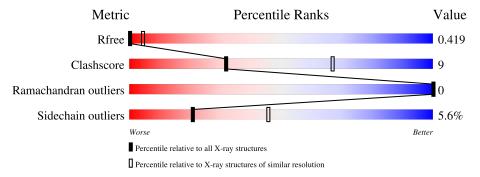
Validation Pipeline (wwPDB-VP) : 2.36

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 8.49 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
R_{free}	130704	1005 (11.50-3.90)		
Clashscore	141614	1070 (11.50-3.90)		
Ramachandran outliers	138981	1003 (11.50-3.90)		
Sidechain outliers	138945	1003 (11.50-3.86)		

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%

Mol	Chain	Length	Quality of chain							
1	A	235	75%		21%					
1	В	235	76%		18%					
2	С	184	57%	30%		11%				
2	D	184	58%	29%	•	11%				



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6229 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	${f Atoms}$				ZeroOcc	AltConf	Trace	
1	Δ	231	Total	С	N	О	S	0	0	0
1	Λ	201	1818	1159	306	338	15	0		
1	D	225	Total	С	N	О	S	0	0	0
1	D	229	1757	1126	292	324	15			

There are 4 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
В	-1	SER	-	expression tag	UNP Q9H9Q4
В	0	GLY	-	expression tag	UNP Q9H9Q4

• Molecule 2 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	164	Total 1327	_	N 224			0	0	0
2	D	164	Total 1327	_	N 224	_	S 6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-19	MET	-	expression tag	UNP Q13426
С	-18	GLY	-	expression tag	UNP Q13426
С	-17	SER	-	expression tag	UNP Q13426
С	-16	SER	-	expression tag	UNP Q13426
С	-15	HIS	-	expression tag	UNP Q13426
С	-14	HIS	-	expression tag	UNP Q13426
С	-13	HIS	-	expression tag	UNP Q13426
С	-12	HIS	-	expression tag	UNP Q13426

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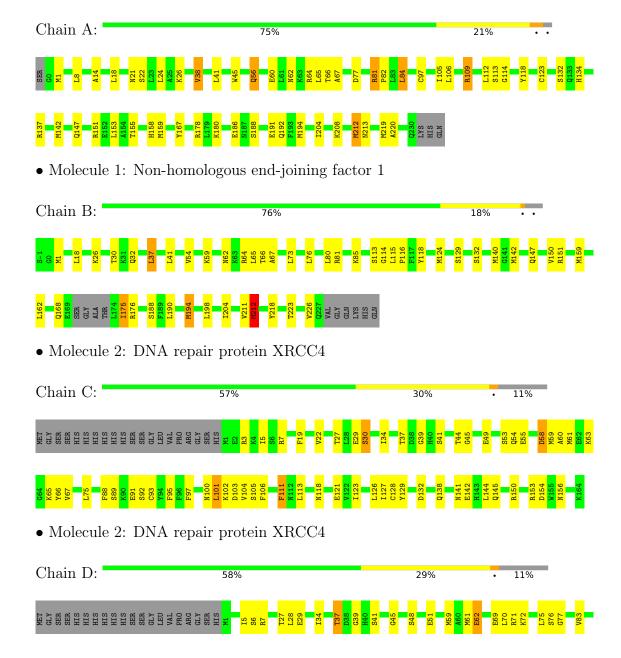
Chain	Residue	Modelled	Actual	Comment	Reference
С	-11	HIS	-	expression tag	UNP Q13426
С	-10	HIS	-	expression tag	UNP Q13426
С	-9	SER	-	expression tag	UNP Q13426
С	-8	SER	-	expression tag	UNP Q13426
С	-7	GLY	-	expression tag	UNP Q13426
С	-6	LEU	-	expression tag	UNP Q13426
С	-5	VAL	-	expression tag	UNP Q13426
С	-4	PRO	-	expression tag	UNP Q13426
С	-3	ARG	-	expression tag	UNP Q13426
С	-2	GLY	-	expression tag	UNP Q13426
С	-1	SER	-	expression tag	UNP Q13426
С	0	HIS	-	expression tag	UNP Q13426
D	-19	MET	-	expression tag	UNP Q13426
D	-18	GLY	-	expression tag	UNP Q13426
D	-17	SER	-	expression tag	UNP Q13426
D	-16	SER	-	expression tag	UNP Q13426
D	-15	HIS	-	expression tag	UNP Q13426
D	-14	HIS	-	expression tag	UNP Q13426
D	-13	HIS	-	expression tag	UNP Q13426
D	-12	HIS	-	expression tag	UNP Q13426
D	-11	HIS	-	expression tag	UNP Q13426
D	-10	HIS	-	expression tag	UNP Q13426
D	-9	SER	-	expression tag	UNP Q13426
D	-8	SER	-	expression tag	UNP Q13426
D	-7	GLY	-	expression tag	UNP Q13426
D	-6	LEU	-	expression tag	UNP Q13426
D	-5	VAL	-	expression tag	UNP Q13426
D	-4	PRO	-	expression tag	UNP Q13426
D	-3	ARG	-	expression tag	UNP Q13426
D	-2	GLY	-	expression tag	UNP Q13426
D	-1	SER	-	expression tag	UNP Q13426
D	0	HIS	-	expression tag	UNP Q13426



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. 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. 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









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	236.76Å 236.76Å 103.23Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.81 - 8.49	Depositor
Resolution (A)	49.81 - 8.49	EDS
% Data completeness	99.3 (49.81-8.49)	Depositor
(in resolution range)	99.9 (49.81-8.49)	EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) > 1$	10.54 (at 8.33Å)	Xtriage
Refinement program	PHENIX (1.7.2_869)	Depositor
Ρ. Р.	0.363 , 0.360	Depositor
R, R_{free}	0.376 , 0.419	DCC
R_{free} test set	149 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	931.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 194.5	EDS
L-test for twinning ²	$< L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	6229	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.34% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.75	6/1854 (0.3%)	0.69	0/2513	
1	В	0.76	7/1793 (0.4%)	0.66	1/2434 (0.0%)	
2	С	0.39	0/1353	0.55	0/1821	
2	D	0.38	0/1353	0.57	0/1821	
All	All	0.63	$13/6353 \ (0.2\%)$	0.63	1/8589 (0.0%)	

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	В	1	MET	CG-SD	6.90	1.99	1.81
1	В	194	MET	CG-SD	6.81	1.98	1.81
1	A	1	MET	CG-SD	6.76	1.98	1.81
1	В	159	MET	CG-SD	6.75	1.98	1.81
1	A	194	MET	CG-SD	6.40	1.97	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	В	37	LEU	CA-CB-CG	5.54	128.03	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	1818	0	1818	29	69
1	В	1757	0	1741	20	25
2	С	1327	0	1290	39	36
2	D	1327	0	1290	33	58
All	All	6229	0	6139	110	94

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.

The worst 5 of 110 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.24	1.02
1:A:62:ASN:HD21	1:A:118:TYR:H	1.20	0.87
2:D:27:THR:HG22	2:D:29:GLU:H	1.39	0.87
2:C:37:THR:HG22	2:C:39:GLY:H	1.39	0.86
2:C:89:SER:HB3	2:C:92:SER:HB3	1.56	0.85

The worst 5 of 94 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	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:64:ARG:NH1	2:C:59:MET:C[6_554]	0.71	1.49
1:B:66:THR:CG2	2:D:105:SER:O[1_556]	0.71	1.49
1:B:65:LEU:CD1	2:D:106:PHE:CE2[1_556]	0.79	1.41
1:A:64:ARG:NE	2:C:59:MET:CB[6_554]	0.88	1.32
1:A:186:GLU:CG	2:D:164:LYS:CD[4_655]	0.93	1.27

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	Perce	ntiles
1	A	$229/235 \ (97\%)$	220 (96%)	9 (4%)	0	100	100
1	В	221/235~(94%)	210 (95%)	11 (5%)	0	100	100
2	C	162/184 (88%)	154 (95%)	8 (5%)	0	100	100
2	D	162/184~(88%)	155~(96%)	7 (4%)	0	100	100
All	All	774/838 (92%)	739 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	entiles
1	A	200/207 (97%)	191 (96%)	9 (4%)	27	52
1	В	191/207 (92%)	179 (94%)	12 (6%)	18	43
2	С	146/163 (90%)	137 (94%)	9 (6%)	18	43
2	D	146/163 (90%)	138 (94%)	8 (6%)	21	47
All	All	683/740 (92%)	645 (94%)	38 (6%)	21	46

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	С	153	ARG
2	D	141	ASN
2	С	156	ASN
2	D	70	LEU
2	D	156	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	141	ASN
2	D	137	ASN
2	С	137	ASN

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Mol	Chain	Res	Type
2	D	118	ASN
2	С	118	ASN

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

