Full wwPDB NMR Structure Validation Report (i)

Feb 24, 2022 – 09:45 AM EST

PDB ID	:	1Z00
Title	:	Solution structure of the C-terminal domain of ERCC1 complexed with the C-terminal domain of XPF
Authors	:	Tripsianes, K.; Folkers, G.; Ab, E.; Das, D.; Odijk, H.; Jaspers, N.G.J.; Hoeijmakers, J.H.J.; Kaptein, R.; Boelens, R.
Deposited on	:	2005-03-01

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

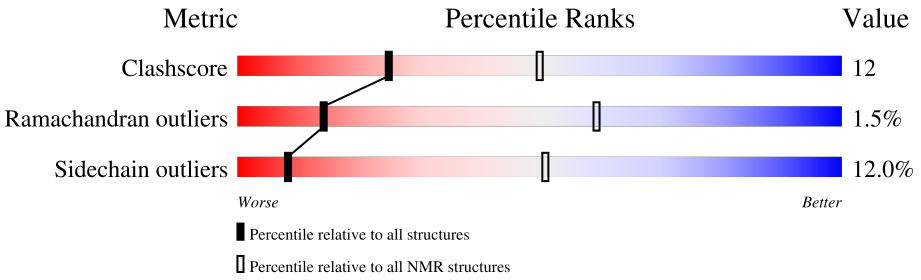
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	89	46% 25% • 21% 6%
2	B	84	49% 20% 5% 26%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:231-A:295, B:833-B:894 (127)	0.15	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 9, 10, 12, 13, 15, 16, 17, 18, 19, 20
2	7, 8, 11, 14

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2614 atoms, of which 1318 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA excision repair protein ERCC-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	84	1319	411	669	110	125	4	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	initiating methionine	UNP P07992
A	298	GLY	-	expression tag	UNP P07992
A	299	GLY	-	expression tag	UNP P07992
A	300	LEU	-	expression tag	UNP P07992
A	301	GLU	-	expression tag	UNP P07992
A	302	HIS	-	expression tag	UNP P07992
A	303	HIS	-	expression tag	UNP P07992
A	304	HIS	-	expression tag	UNP P07992
A	305	HIS	-	expression tag	UNP P07992
A	306	HIS	-	expression tag	UNP P07992
A	307	HIS	-	expression tag	UNP P07992

- Molecule 2 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	84	1295	405	649	111	126	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	822	MET	-	initiating methionine	UNP Q92889

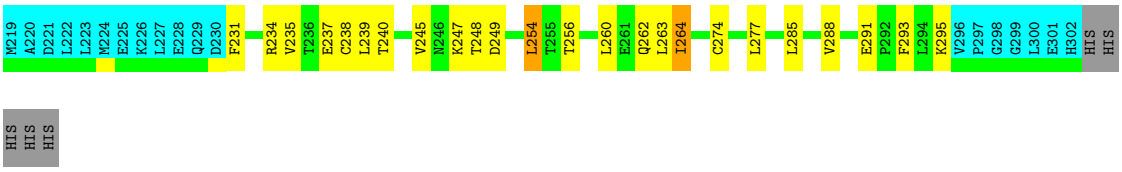
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 46% 25% • 21% 6%



• Molecule 2: DNA repair endonuclease XPF

Chain B: 49% 20% 5% 26%

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 44% 27% • 21% 6%

• Molecule 2: DNA repair endonuclease XPF

Chain B: 50% 19% 5% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 F840 L841 L842 K843 M844 P845 C852 L855 V859 K860 N861 I862 A863 Q870 L873 A883 K884 D888 T892 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.2 Score per residue for model 2

- Molecule 1: DNA excision repair protein ERCC-1

Chain A: 42% 29% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 R234 V235 T236 E237 C238 L239 T240 K243 K247 T248 D249 T252 L253 L254 T255 T256 L260 E261 Q262 L263 I264 R268 E269 D270 C274 L285 F286 D287 V288 L289 H290 E291 P292 F293 L294 K295 V296 P297 G298 G299

L300 E301 H302 HIS HIS HIS HIS HIS

- Molecule 2: DNA repair endonuclease XPF

Chain B: 48% 20% 6% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 N834 P835 Q838 D839 F840 L841 L842 K843 C852 L855 V859 K860 N861 I862 Q870 L873 N879 A880 A881 N882 A883 K884 Q885 L886 I890 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.3 Score per residue for model 3

- Molecule 1: DNA excision repair protein ERCC-1

Chain A: 42% 27% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 F231 R234 V235 T236 E237 C238 L239 T240 V245 N246 K247 T248 D249 L254 T255 T256 L260 E261 Q262 L263 I264 L271 C274 L277 G278 P279 Q280 K281 A282 R283 R284 L285 V288 E291 P292 K295 V296 P297

G298 G299 L300 E301 H302 HIS HIS HIS HIS HIS

- Molecule 2: DNA repair endonuclease XPF

Chain B: 49% 20% 5% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 F840 L841 P845 C852 L855 V859 K860 N861 I862 A863 E864 L868 S869 Q870 L873 A883 L886 F889 T892 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.4 Score per residue for model 4

- Molecule 1: DNA excision repair protein ERCC-1

Chain A: 43% 28% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 F231 R234 V235 T236 E237 C238 L239 T240 N246 K247 T248 D249 L254 T255 T256 L260 E261 Q262 L263 I264 R268 C274 P275 G276 L277 G278 P279 R283 R284 L285 F286 D287 V288 L289 F293 L294 K295 V296 P297 G298

G299 L300 E301 H302 HIS HIS HIS HIS HIS

• Molecule 2: DNA repair endonuclease XPF

Chain B: 50% 20% • 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 F840 L841 L842 K843 M844 P845 N848 C852 L855 V859 K860 N861 I862 A863 E864 L868 S869 Q870 L873 A883 T892 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.5 Score per residue for model 5

• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 43% 28% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 F231 R234 V235 T236 E237 C238 L239 T240 K243 S244 V245 N246 K247 T248 D249 L254 T255 T256 L260 E261 Q262 L263 I264 C274 P275 G276 L277 G278 P279 R283 D287 V288 E291 K295 V296 P297 G298 G299 L300

E301 H302 HIS HIS HIS HIS HIS

• Molecule 2: DNA repair endonuclease XPF

Chain B: 49% 20% 5% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 F840 L841 L842 K843 N851 C852 L855 V859 K860 N861 I862 A863 E864 L868 S869 Q870 L873 L877 A883 K884 Q885 L886 T892 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.6 Score per residue for model 6

• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 49% 20% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 S233 R234 V235 T236 E237 C238 L239 T240 V245 N246 K247 T248 D249 L254 L260 E261 Q262 L263 I264 R268 C274 P275 G276 L277 F286 K295 V296 P297 G298 G299 L300 E301 H302 HIS HIS HIS HIS HIS

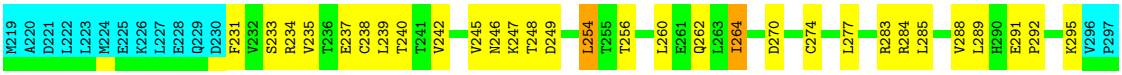
• Molecule 2: DNA repair endonuclease XPF

Chain B: 49% 23% • 26%

4.2.7 Score per residue for model 7

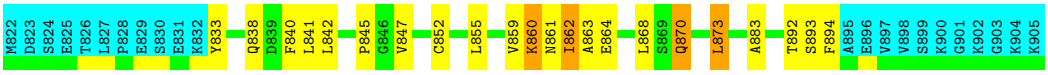
• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



• Molecule 2: DNA repair endonuclease XPF

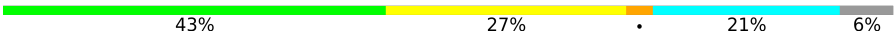
Chain B:

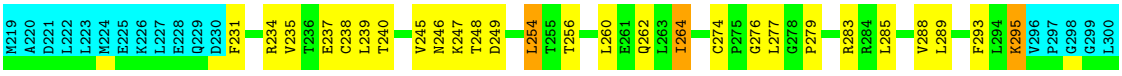


4.2.8 Score per residue for model 8

• Molecule 1: DNA excision repair protein ERCC-1

Chain A:





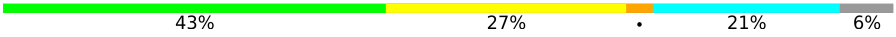
• Molecule 2: DNA repair endonuclease XPF

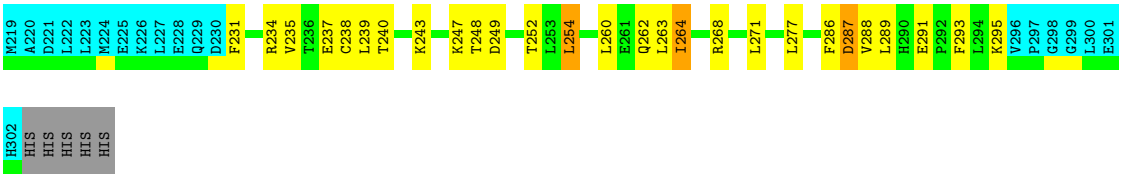
Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: DNA excision repair protein ERCC-1

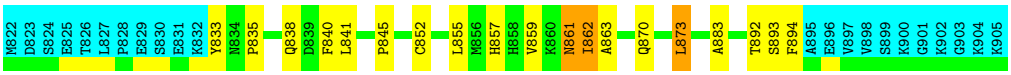
Chain A:





• Molecule 2: DNA repair endonuclease XPF

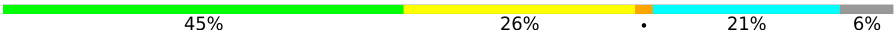
Chain B:

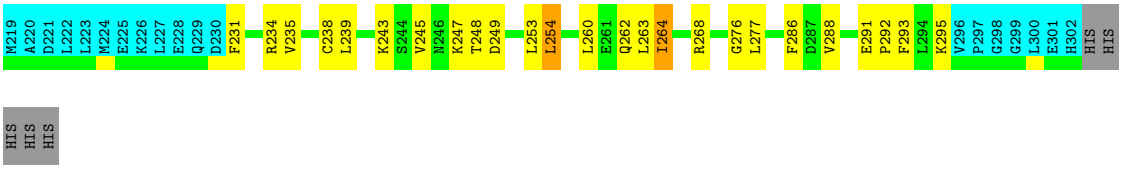


4.2.10 Score per residue for model 10

• Molecule 1: DNA excision repair protein ERCC-1

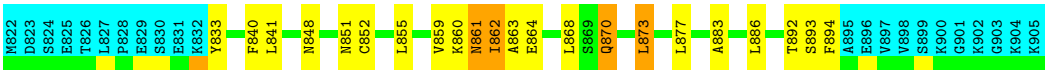
Chain A:





• Molecule 2: DNA repair endonuclease XPF

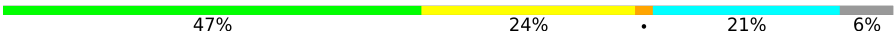
Chain B:

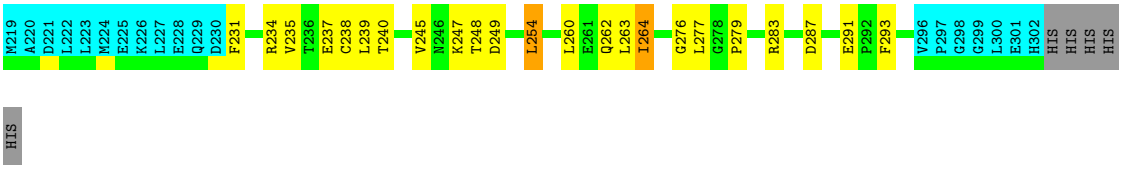


4.2.11 Score per residue for model 11

• Molecule 1: DNA excision repair protein ERCC-1

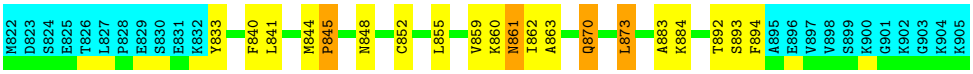
Chain A:





• Molecule 2: DNA repair endonuclease XPF

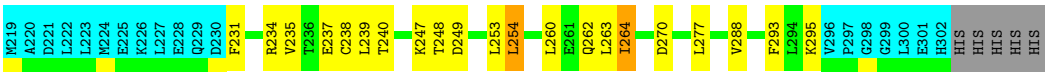
Chain B:



4.2.12 Score per residue for model 12

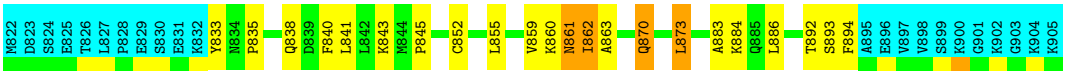
• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



• Molecule 2: DNA repair endonuclease XPF

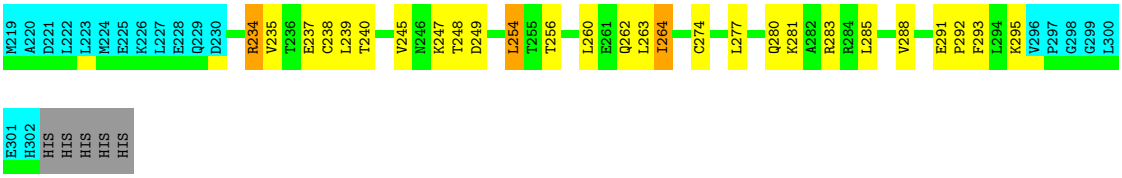
Chain B:



4.2.13 Score per residue for model 13

• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



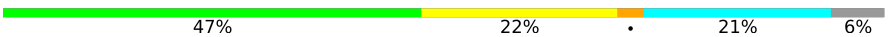
• Molecule 2: DNA repair endonuclease XPF

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



HIS

• Molecule 2: DNA repair endonuclease XPF

Chain B: 45% 24% 5% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 Q838 D839 F840 L841 L842 K843 M844 P845 G846 V847 C852 L855 V859 K860 N861 I862 A863 E864 L868 S869 Q870 L873 A883 L886 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 48% 22% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 F231 R234 V235 T236 E237 C238 L239 T240 V245 N246 K247 T248 D249 L254 L260 E261 Q262 L263 I264 R268 L277 K281 L285 F286 D287 V288 F293 V296 P297 G298 G299 L300 E301 H302 HIS HIS HIS HIS

HIS

• Molecule 2: DNA repair endonuclease XPF

Chain B: 46% 23% 5% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 D839 F840 L841 L842 K843 N848 N851 C852 L855 V859 K860 N861 I862 A863 E864 L868 S869 Q870 L873 L877 A883 L886 T892 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.16 Score per residue for model 16

• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 39% 30% • 21% 6%

M219 A220 D221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 F231 R234 V235 T236 E237 C238 L239 T240 K243 S244 V245 N246 K247 T248 D249 S250 L253 L254 T255 T256 L260 E261 Q262 L263 I264 S267 R268 F269 D270 G274 L277 K281 F286 D287 V288 F293 L294 K295

V296 P297 G298 G299 L300 E301 H302 HIS HIS HIS HIS HIS

• Molecule 2: DNA repair endonuclease XPF

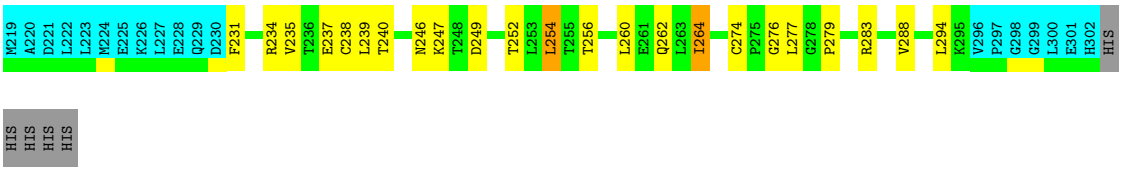
Chain B: 45% 24% 5% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 Y833 F840 L841 P845 N848 N851 C852 L855 V859 K860 N861 I862 A863 Q870 L873 L877 G878 N879 A880 A881 N882 A883 L886 F889 I890 H891 T892 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903

4.2.17 Score per residue for model 17

• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



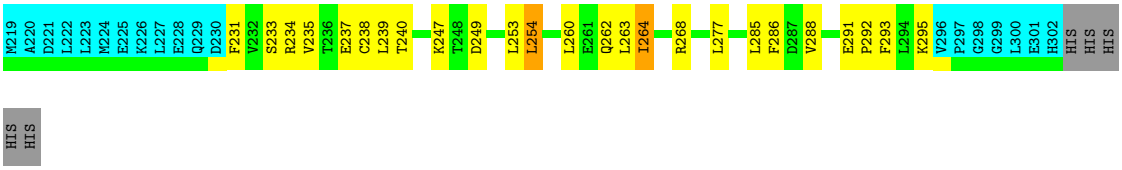
• Molecule 2: DNA repair endonuclease XPF

Chain B:

4.2.18 Score per residue for model 18

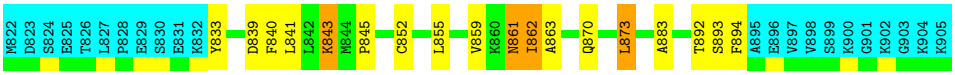
• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



• Molecule 2: DNA repair endonuclease XPF

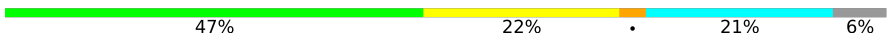
Chain B:

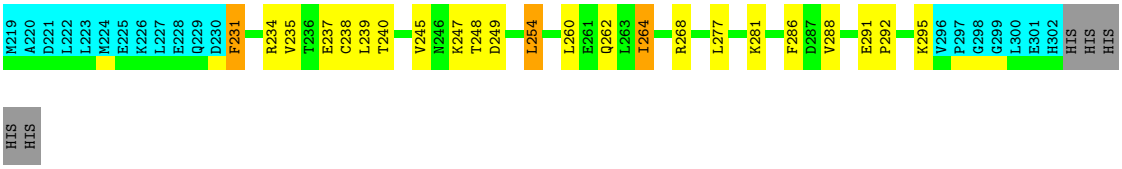


4.2.19 Score per residue for model 19

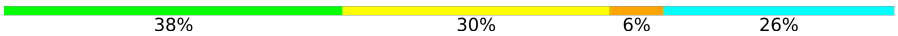
• Molecule 1: DNA excision repair protein ERCC-1

Chain A:



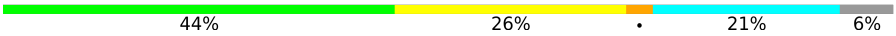


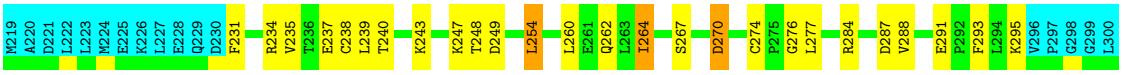
• Molecule 2: DNA repair endonuclease XPF

Chain B: 

4.2.20 Score per residue for model 20

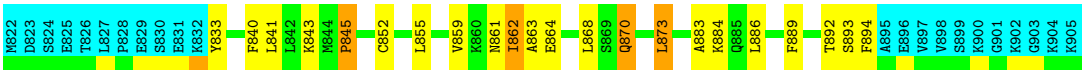
• Molecule 1: DNA excision repair protein ERCC-1

Chain A: 



• Molecule 2: DNA repair endonuclease XPF

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *water refinment in CNS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.0
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	234	ARG	Sidechain	2
1	A	283	ARG	Sidechain	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	504	524	524	15±2
2	B	481	476	476	14±1
All	All	19700	20000	20000	461

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 12.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:873:LEU:HD13	2:B:883:ALA:HB1	0.72	1.60	17	20
2:B:838:GLN:O	2:B:842:LEU:HG	0.70	1.87	7	2
1:A:235:VAL:O	1:A:239:LEU:HG	0.64	1.93	15	20
1:A:254:LEU:HD22	2:B:894:PHE:CZ	0.62	2.30	19	18
1:A:249:ASP:OD1	1:A:277:LEU:HD13	0.61	1.96	18	19
2:B:864:GLU:O	2:B:868:LEU:HG	0.59	1.97	4	12
2:B:835:PRO:HA	2:B:838:GLN:OE1	0.58	1.98	19	1
2:B:841:LEU:HG	2:B:852:CYS:SG	0.57	2.39	10	17
2:B:855:LEU:O	2:B:859:VAL:HG12	0.57	1.99	9	20
1:A:235:VAL:HG12	1:A:260:LEU:HD23	0.56	1.77	15	14
2:B:873:LEU:CD1	2:B:883:ALA:HB1	0.56	2.30	7	20
1:A:231:PHE:CE2	2:B:892:THR:HG23	0.53	2.39	4	16
1:A:238:CYS:HB3	2:B:840:PHE:CZ	0.52	2.39	12	20
1:A:237:GLU:HA	1:A:240:THR:OG1	0.52	2.05	13	19
1:A:293:PHE:CE2	2:B:861:ASN:HA	0.52	2.39	16	12
2:B:847:VAL:HG12	2:B:852:CYS:SG	0.52	2.45	7	3
1:A:254:LEU:HD13	2:B:894:PHE:CE1	0.51	2.40	12	3
1:A:245:VAL:HG13	1:A:249:ASP:HB3	0.51	1.83	3	12
1:A:284:ARG:HA	1:A:287:ASP:OD2	0.51	2.06	20	1
1:A:287:ASP:O	1:A:291:GLU:HB2	0.50	2.06	5	5
1:A:260:LEU:O	1:A:264:ILE:HG22	0.50	2.06	12	20
1:A:291:GLU:OE2	1:A:292:PRO:HD2	0.50	2.06	13	5
1:A:279:PRO:O	1:A:283:ARG:HD3	0.50	2.07	11	7
1:A:231:PHE:CD2	2:B:894:PHE:HB3	0.49	2.42	12	3
1:A:256:THR:HG21	1:A:274:CYS:SG	0.49	2.47	7	11
1:A:264:ILE:HD11	2:B:863:ALA:HA	0.49	1.85	5	19
1:A:284:ARG:O	1:A:288:VAL:HG23	0.48	2.07	7	1
2:B:841:LEU:HD11	2:B:855:LEU:HD12	0.48	1.86	9	17
2:B:870:GLN:HA	2:B:873:LEU:HD11	0.48	1.85	10	15
1:A:268:ARG:HG3	1:A:286:PHE:CD1	0.48	2.44	15	3
1:A:254:LEU:HD22	2:B:894:PHE:CE1	0.48	2.43	16	4
1:A:285:LEU:HD12	1:A:288:VAL:CG2	0.48	2.39	13	4
1:A:249:ASP:CG	1:A:277:LEU:HD13	0.47	2.28	15	5
1:A:253:LEU:HD21	1:A:277:LEU:HD22	0.47	1.85	18	3
2:B:845:PRO:HG3	2:B:889:PHE:CG	0.47	2.45	3	5
1:A:289:LEU:HA	2:B:862:ILE:CD1	0.47	2.39	7	5
2:B:839:ASP:O	2:B:843:LYS:HG2	0.47	2.09	2	4
1:A:288:VAL:O	2:B:862:ILE:HD11	0.46	2.10	2	17
1:A:242:VAL:CG1	1:A:288:VAL:HG21	0.46	2.41	7	1
1:A:268:ARG:HG3	1:A:286:PHE:CD2	0.46	2.46	18	6
2:B:860:LYS:HD3	2:B:860:LYS:C	0.45	2.32	17	1
1:A:271:LEU:O	1:A:277:LEU:HD23	0.45	2.12	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:292:PRO:HA	2:B:860:LYS:O	0.45	2.11	7	1
2:B:886:LEU:O	2:B:890:ILE:HG13	0.44	2.11	19	2
1:A:245:VAL:HG21	1:A:285:LEU:HD23	0.44	1.87	3	2
1:A:274:CYS:SG	1:A:277:LEU:HB2	0.44	2.52	6	1
1:A:280:GLN:HG3	1:A:281:LYS:N	0.44	2.28	13	1
1:A:291:GLU:OE1	1:A:292:PRO:HD2	0.44	2.13	18	1
1:A:293:PHE:CZ	2:B:841:LEU:HD22	0.43	2.48	18	5
2:B:835:PRO:HA	2:B:838:GLN:HG2	0.43	1.89	9	3
2:B:851:ASN:HB3	2:B:877:LEU:CD2	0.43	2.44	19	4
1:A:235:VAL:HG11	2:B:894:PHE:CE2	0.43	2.49	15	1
2:B:884:LYS:O	2:B:888:ASP:HB2	0.42	2.13	1	1
1:A:267:SER:O	1:A:270:ASP:HB2	0.42	2.15	20	2
1:A:277:LEU:HD11	1:A:281:LYS:HB2	0.42	1.91	3	4
2:B:851:ASN:HB3	2:B:877:LEU:HD22	0.42	1.91	16	1
1:A:260:LEU:HB3	2:B:890:ILE:HA	0.42	1.92	2	1
2:B:842:LEU:HA	2:B:852:CYS:SG	0.42	2.54	14	2
2:B:884:LYS:C	2:B:884:LYS:HD3	0.42	2.35	11	2
2:B:844:MET:SD	2:B:845:PRO:HD2	0.41	2.56	11	1
1:A:249:ASP:O	1:A:253:LEU:HG	0.41	2.15	10	1
1:A:249:ASP:O	1:A:252:THR:HB	0.41	2.16	17	3
2:B:879:ASN:OD1	2:B:881:ALA:HB3	0.41	2.16	16	1
1:A:237:GLU:OE1	2:B:843:LYS:HE3	0.41	2.16	2	1
1:A:295:LYS:HG3	2:B:834:ASN:OD1	0.41	2.15	8	1
1:A:243:LYS:HA	1:A:243:LYS:HE3	0.41	1.93	10	1
2:B:881:ALA:O	2:B:885:GLN:HG3	0.40	2.16	2	2
2:B:884:LYS:HD3	2:B:884:LYS:C	0.40	2.37	13	1
1:A:294:LEU:HD22	2:B:833:TYR:CZ	0.40	2.51	17	1
1:A:247:LYS:HA	1:A:250:SER:OG	0.40	2.17	16	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	65/89 (73%)	60±1 (93±1%)	3±1 (5±2%)	1±1 (2±1%)	11 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	62/84 (74%)	60±1 (97±1%)	1±1 (2±1%)	1±0 (1±1%)	20	68
All	All	2540/3460 (73%)	2404 (95%)	97 (4%)	39 (2%)	14	59

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	295	LYS	16
2	B	845	PRO	13
1	A	276	GLY	9
1	A	275	PRO	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	58/79 (73%)	51±1 (88±2%)	7±1 (12±2%)	9	52
2	B	52/71 (73%)	46±1 (88±3%)	6±1 (12±3%)	8	50
All	All	2200/3000 (73%)	1936 (88%)	264 (12%)	8	51

All 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	247	LYS	20
1	A	254	LEU	20
1	A	262	GLN	20
1	A	264	ILE	20
2	B	861	ASN	20
2	B	870	GLN	20
2	B	873	LEU	20
2	B	862	ILE	19
1	A	248	THR	16
1	A	263	LEU	11
2	B	843	LYS	11
2	B	860	LYS	11

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Mol	Chain	Res	Type	Models (Total)
2	B	886	LEU	11
2	B	848	ASN	8
1	A	243	LYS	6
1	A	285	LEU	5
1	A	270	ASP	4
1	A	246	ASN	4
2	B	884	LYS	4
2	B	864	GLU	3
2	B	888	ASP	2
1	A	274	CYS	2
1	A	283	ARG	2
1	A	287	ASP	2
1	A	231	PHE	2
2	B	879	ASN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided