



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 03:23 PM UTC

PDB ID : 3RWR / pdb_00003rwr
Title : Crystal structure of the human XRCC4-XLF complex
Authors : Andres, S.N.; Junop, M.S.
Deposited on : 2011-05-09
Resolution : 3.94 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

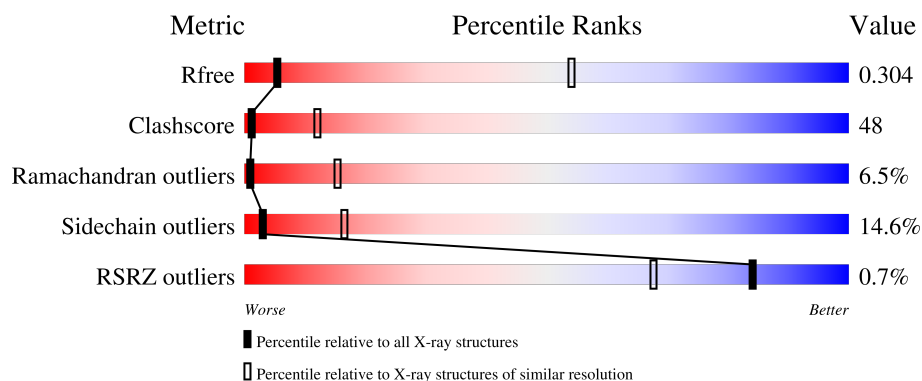
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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}	180053	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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 $\leq 5\%$. 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	163	26% 52% 10% • 10%
1	B	163	% 33% 44% 15% • 7%
1	F	163	% 36% 49% 12% •
1	G	163	% 34% 52% 10% •
1	J	163	2% 39% 45% 12% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	163	
1	N	163	
1	P	163	
1	R	163	
1	U	163	
1	V	163	
1	Y	163	
2	D	230	
2	E	230	
2	H	230	
2	I	230	
2	L	230	
2	M	230	
2	O	230	
2	Q	230	
2	S	230	
2	T	230	
2	W	230	
2	X	230	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	J	164	-	-	X	-
3	TBR	P	2	-	-	X	-
3	TBR	X	5	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36833 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 DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1171	741	193	231	6			
1	B	152	Total	C	N	O	S	0	0	0
			1239	782	207	244	6			
1	F	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	G	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	J	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	K	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	N	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	P	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	R	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	V	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	U	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	Y	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	HIS	-	expression tag	UNP Q13426
A	159	HIS	-	expression tag	UNP Q13426
A	160	HIS	-	expression tag	UNP Q13426
A	161	HIS	-	expression tag	UNP Q13426
A	162	HIS	-	expression tag	UNP Q13426

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	HIS	-	expression tag	UNP Q13426
B	658	HIS	-	expression tag	UNP Q13426
B	659	HIS	-	expression tag	UNP Q13426
B	660	HIS	-	expression tag	UNP Q13426
B	661	HIS	-	expression tag	UNP Q13426
B	662	HIS	-	expression tag	UNP Q13426
B	663	HIS	-	expression tag	UNP Q13426
F	158	HIS	-	expression tag	UNP Q13426
F	159	HIS	-	expression tag	UNP Q13426
F	160	HIS	-	expression tag	UNP Q13426
F	161	HIS	-	expression tag	UNP Q13426
F	162	HIS	-	expression tag	UNP Q13426
F	163	HIS	-	expression tag	UNP Q13426
G	658	HIS	-	expression tag	UNP Q13426
G	659	HIS	-	expression tag	UNP Q13426
G	660	HIS	-	expression tag	UNP Q13426
G	661	HIS	-	expression tag	UNP Q13426
G	662	HIS	-	expression tag	UNP Q13426
G	663	HIS	-	expression tag	UNP Q13426
J	158	HIS	-	expression tag	UNP Q13426
J	159	HIS	-	expression tag	UNP Q13426
J	160	HIS	-	expression tag	UNP Q13426
J	161	HIS	-	expression tag	UNP Q13426
J	162	HIS	-	expression tag	UNP Q13426
J	163	HIS	-	expression tag	UNP Q13426
K	658	HIS	-	expression tag	UNP Q13426
K	659	HIS	-	expression tag	UNP Q13426
K	660	HIS	-	expression tag	UNP Q13426
K	661	HIS	-	expression tag	UNP Q13426
K	662	HIS	-	expression tag	UNP Q13426
K	663	HIS	-	expression tag	UNP Q13426
N	158	HIS	-	expression tag	UNP Q13426
N	159	HIS	-	expression tag	UNP Q13426
N	160	HIS	-	expression tag	UNP Q13426
N	161	HIS	-	expression tag	UNP Q13426
N	162	HIS	-	expression tag	UNP Q13426
N	163	HIS	-	expression tag	UNP Q13426
P	658	HIS	-	expression tag	UNP Q13426
P	659	HIS	-	expression tag	UNP Q13426
P	660	HIS	-	expression tag	UNP Q13426
P	661	HIS	-	expression tag	UNP Q13426
P	662	HIS	-	expression tag	UNP Q13426

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	663	HIS	-	expression tag	UNP Q13426
R	158	HIS	-	expression tag	UNP Q13426
R	159	HIS	-	expression tag	UNP Q13426
R	160	HIS	-	expression tag	UNP Q13426
R	161	HIS	-	expression tag	UNP Q13426
R	162	HIS	-	expression tag	UNP Q13426
R	163	HIS	-	expression tag	UNP Q13426
V	658	HIS	-	expression tag	UNP Q13426
V	659	HIS	-	expression tag	UNP Q13426
V	660	HIS	-	expression tag	UNP Q13426
V	661	HIS	-	expression tag	UNP Q13426
V	662	HIS	-	expression tag	UNP Q13426
V	663	HIS	-	expression tag	UNP Q13426
U	158	HIS	-	expression tag	UNP Q13426
U	159	HIS	-	expression tag	UNP Q13426
U	160	HIS	-	expression tag	UNP Q13426
U	161	HIS	-	expression tag	UNP Q13426
U	162	HIS	-	expression tag	UNP Q13426
U	163	HIS	-	expression tag	UNP Q13426
Y	658	HIS	-	expression tag	UNP Q13426
Y	659	HIS	-	expression tag	UNP Q13426
Y	660	HIS	-	expression tag	UNP Q13426
Y	661	HIS	-	expression tag	UNP Q13426
Y	662	HIS	-	expression tag	UNP Q13426
Y	663	HIS	-	expression tag	UNP Q13426

- Molecule 2 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	E	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	H	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	I	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	L	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	M	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	O	227	Total	C	N	O	S	0	0	0
			1807	1153	306	333	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	S	218	Total	C	N	O	S	0	0	0
			1744	1115	295	319	15			
2	W	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	T	224	Total	C	N	O	S	0	0	0
			1789	1142	302	330	15			
2	X	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	225	HIS	-	expression tag	UNP Q9H9Q4
D	226	HIS	-	expression tag	UNP Q9H9Q4
D	227	HIS	-	expression tag	UNP Q9H9Q4
D	228	HIS	-	expression tag	UNP Q9H9Q4
D	229	HIS	-	expression tag	UNP Q9H9Q4
D	230	HIS	-	expression tag	UNP Q9H9Q4
E	725	HIS	-	expression tag	UNP Q9H9Q4
E	726	HIS	-	expression tag	UNP Q9H9Q4
E	727	HIS	-	expression tag	UNP Q9H9Q4
E	728	HIS	-	expression tag	UNP Q9H9Q4
E	729	HIS	-	expression tag	UNP Q9H9Q4
E	730	HIS	-	expression tag	UNP Q9H9Q4
H	225	HIS	-	expression tag	UNP Q9H9Q4
H	226	HIS	-	expression tag	UNP Q9H9Q4
H	227	HIS	-	expression tag	UNP Q9H9Q4
H	228	HIS	-	expression tag	UNP Q9H9Q4
H	229	HIS	-	expression tag	UNP Q9H9Q4
H	230	HIS	-	expression tag	UNP Q9H9Q4
I	725	HIS	-	expression tag	UNP Q9H9Q4
I	726	HIS	-	expression tag	UNP Q9H9Q4
I	727	HIS	-	expression tag	UNP Q9H9Q4
I	728	HIS	-	expression tag	UNP Q9H9Q4
I	729	HIS	-	expression tag	UNP Q9H9Q4
I	730	HIS	-	expression tag	UNP Q9H9Q4
L	225	HIS	-	expression tag	UNP Q9H9Q4
L	226	HIS	-	expression tag	UNP Q9H9Q4
L	227	HIS	-	expression tag	UNP Q9H9Q4
L	228	HIS	-	expression tag	UNP Q9H9Q4
L	229	HIS	-	expression tag	UNP Q9H9Q4

Continued on next page...

Continued from previous page...

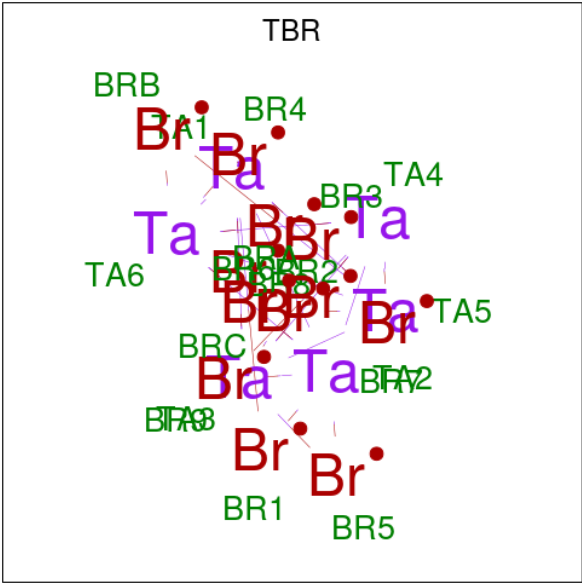
Chain	Residue	Modelled	Actual	Comment	Reference
L	230	HIS	-	expression tag	UNP Q9H9Q4
M	725	HIS	-	expression tag	UNP Q9H9Q4
M	726	HIS	-	expression tag	UNP Q9H9Q4
M	727	HIS	-	expression tag	UNP Q9H9Q4
M	728	HIS	-	expression tag	UNP Q9H9Q4
M	729	HIS	-	expression tag	UNP Q9H9Q4
M	730	HIS	-	expression tag	UNP Q9H9Q4
O	225	HIS	-	expression tag	UNP Q9H9Q4
O	226	HIS	-	expression tag	UNP Q9H9Q4
O	227	HIS	-	expression tag	UNP Q9H9Q4
O	228	HIS	-	expression tag	UNP Q9H9Q4
O	229	HIS	-	expression tag	UNP Q9H9Q4
O	230	HIS	-	expression tag	UNP Q9H9Q4
Q	725	HIS	-	expression tag	UNP Q9H9Q4
Q	726	HIS	-	expression tag	UNP Q9H9Q4
Q	727	HIS	-	expression tag	UNP Q9H9Q4
Q	728	HIS	-	expression tag	UNP Q9H9Q4
Q	729	HIS	-	expression tag	UNP Q9H9Q4
Q	730	HIS	-	expression tag	UNP Q9H9Q4
S	225	HIS	-	expression tag	UNP Q9H9Q4
S	226	HIS	-	expression tag	UNP Q9H9Q4
S	227	HIS	-	expression tag	UNP Q9H9Q4
S	228	HIS	-	expression tag	UNP Q9H9Q4
S	229	HIS	-	expression tag	UNP Q9H9Q4
S	230	HIS	-	expression tag	UNP Q9H9Q4
W	725	HIS	-	expression tag	UNP Q9H9Q4
W	726	HIS	-	expression tag	UNP Q9H9Q4
W	727	HIS	-	expression tag	UNP Q9H9Q4
W	728	HIS	-	expression tag	UNP Q9H9Q4
W	729	HIS	-	expression tag	UNP Q9H9Q4
W	730	HIS	-	expression tag	UNP Q9H9Q4
T	225	HIS	-	expression tag	UNP Q9H9Q4
T	226	HIS	-	expression tag	UNP Q9H9Q4
T	227	HIS	-	expression tag	UNP Q9H9Q4
T	228	HIS	-	expression tag	UNP Q9H9Q4
T	229	HIS	-	expression tag	UNP Q9H9Q4
T	230	HIS	-	expression tag	UNP Q9H9Q4
X	725	HIS	-	expression tag	UNP Q9H9Q4
X	726	HIS	-	expression tag	UNP Q9H9Q4
X	727	HIS	-	expression tag	UNP Q9H9Q4
X	728	HIS	-	expression tag	UNP Q9H9Q4
X	729	HIS	-	expression tag	UNP Q9H9Q4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	730	HIS	-	expression tag	UNP Q9H9Q4

- Molecule 3 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).

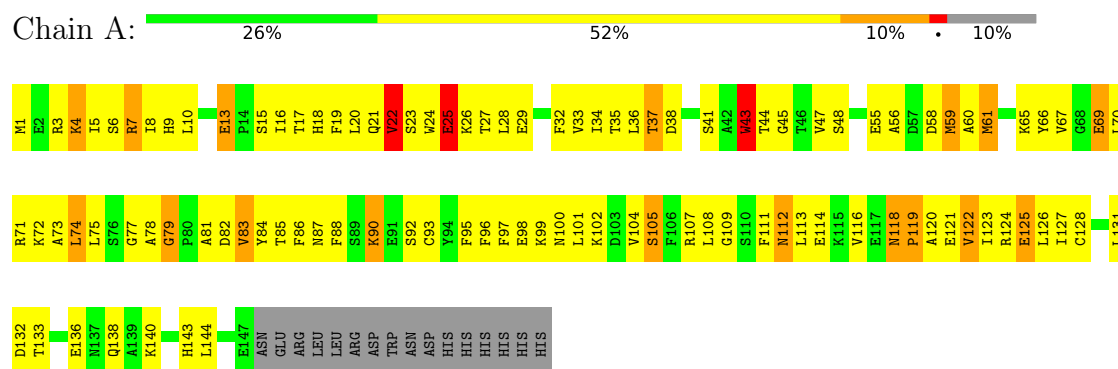


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	H	1	Total	Br	Ta	0	0
			18	12	6		
3	J	1	Total	Br	Ta	0	0
			18	12	6		
3	M	1	Total	Br	Ta	0	0
			18	12	6		
3	P	1	Total	Br	Ta	0	0
			18	12	6		
3	V	1	Total	Br	Ta	0	0
			18	12	6		
3	X	1	Total	Br	Ta	0	0
			18	12	6		
3	Y	1	Total	Br	Ta	0	0
			18	12	6		

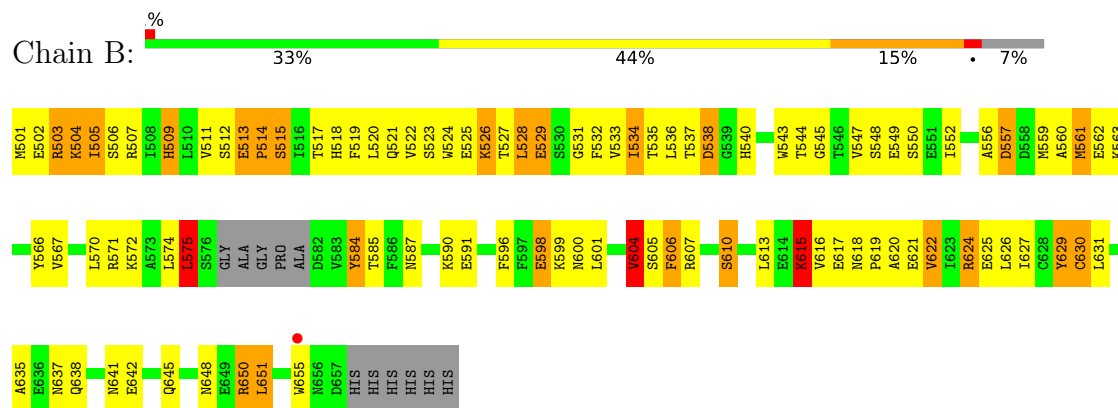
3 Residue-property plots

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.

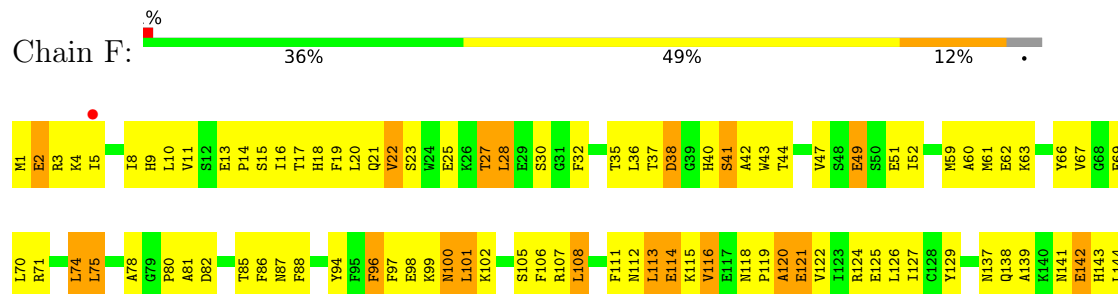
• Molecule 1: DNA repair protein XRCC4



• Molecule 1: DNA repair protein XRCC4

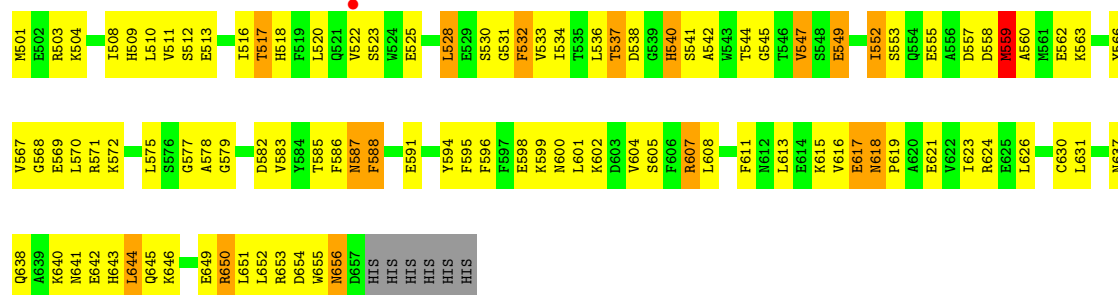


• Molecule 1: DNA repair protein XRCC4

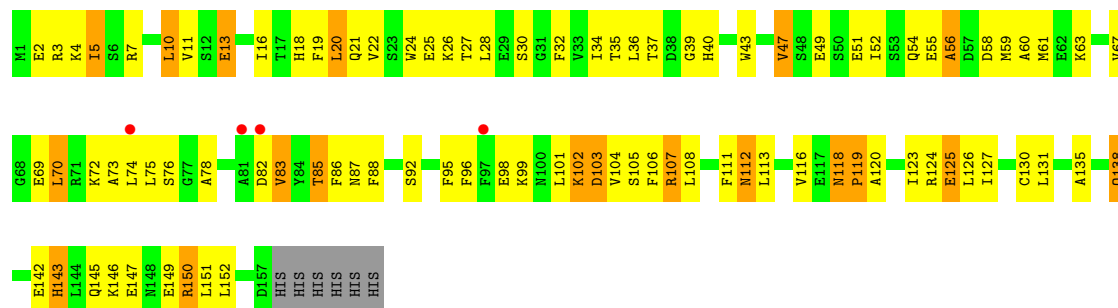




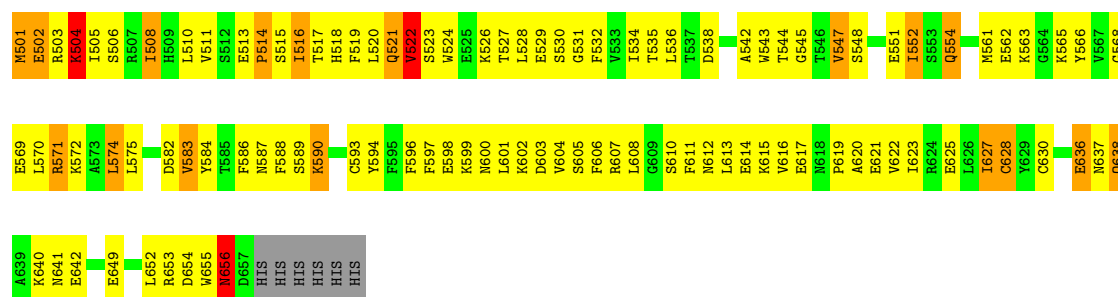
• Molecule 1: DNA repair protein XRCC4



• Molecule 1: DNA repair protein XRCC4

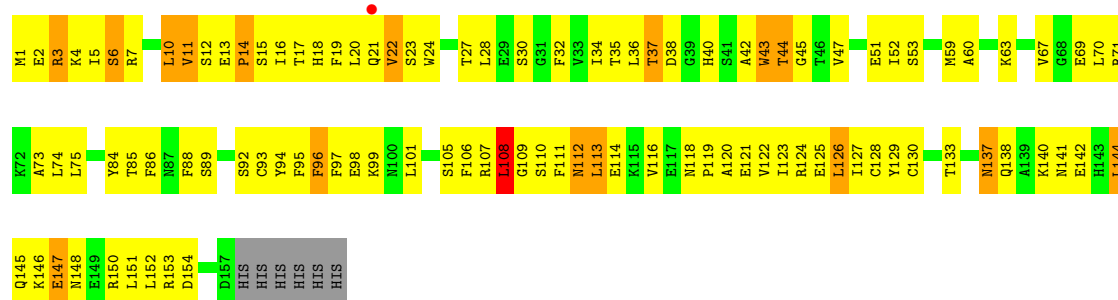


• Molecule 1: DNA repair protein XRCC4

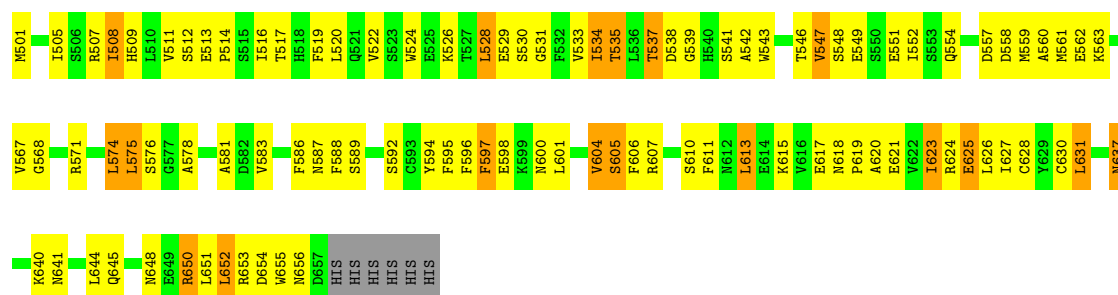


• Molecule 1: DNA repair protein XRCC4

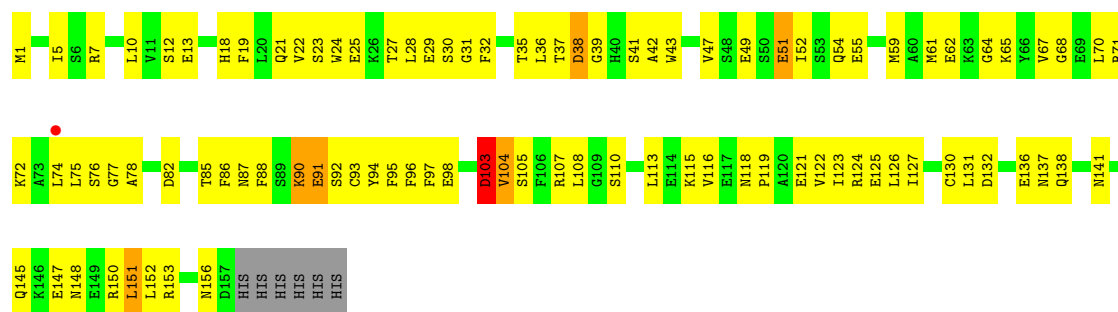




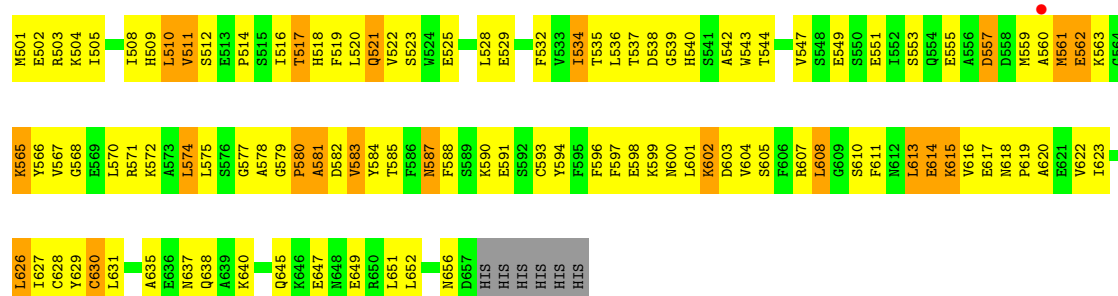
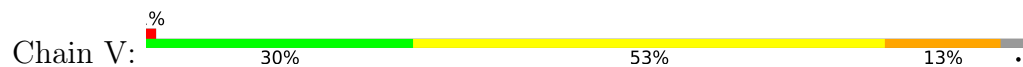
• Molecule 1: DNA repair protein XRCC4



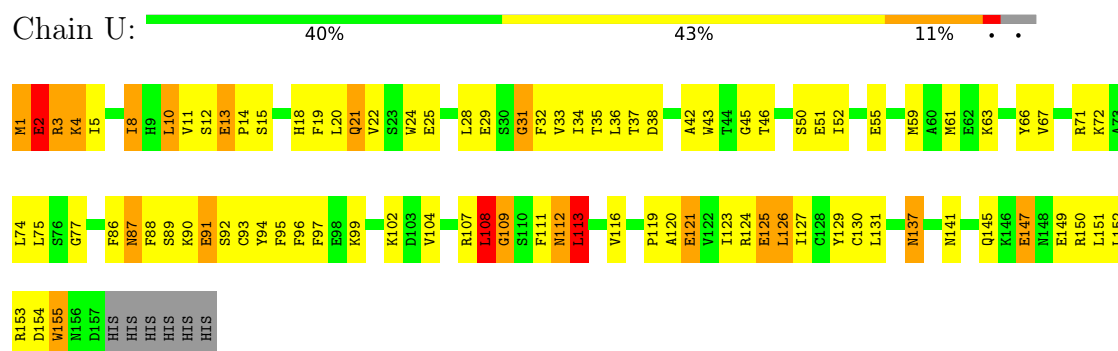
• Molecule 1: DNA repair protein XRCC4



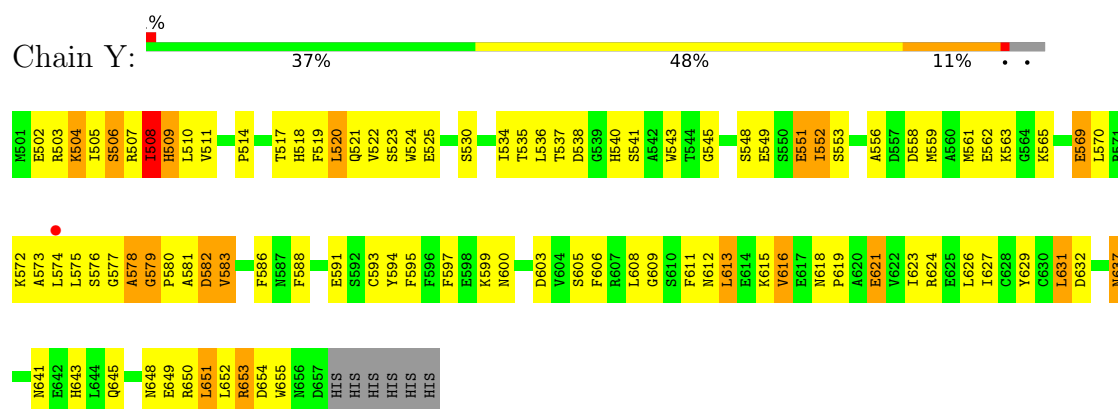
• Molecule 1: DNA repair protein XRCC4



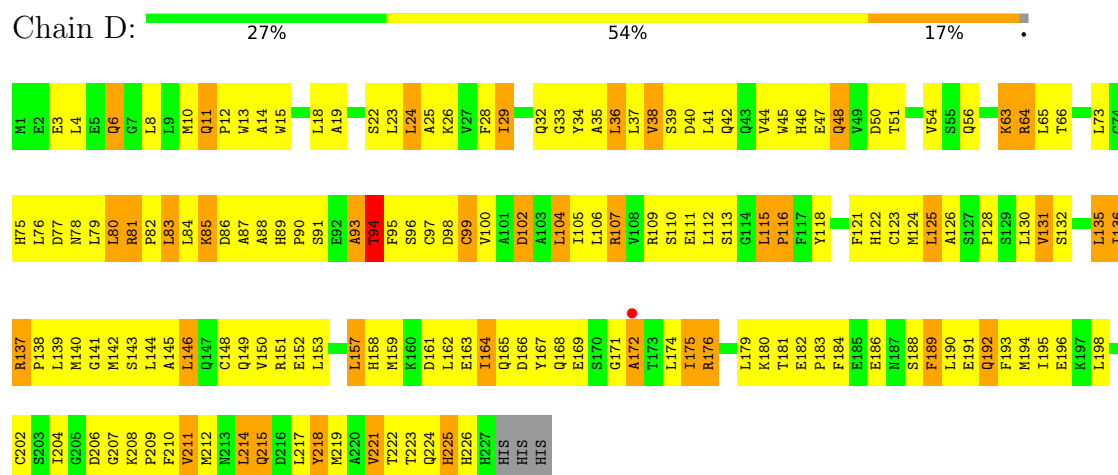
- Molecule 1: DNA repair protein XRCC4



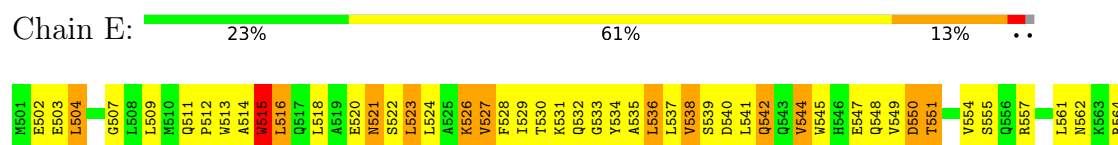
- Molecule 1: DNA repair protein XRCC4

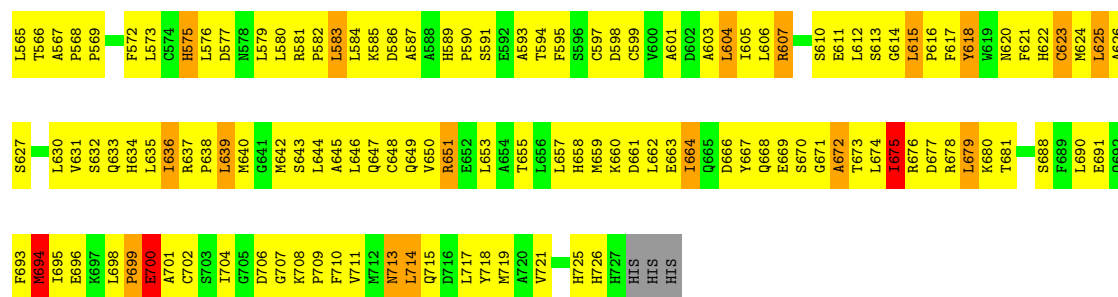


- Molecule 2: Non-homologous end-joining factor 1



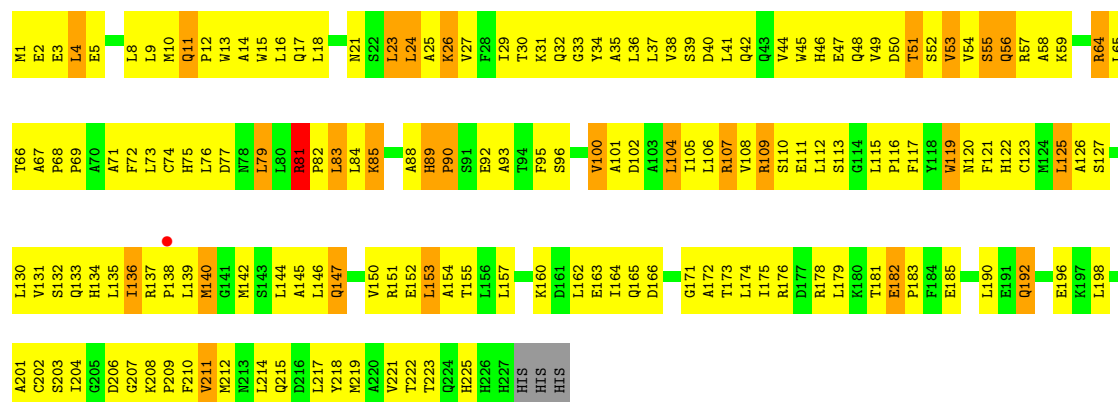
- Molecule 2: Non-homologous end-joining factor 1





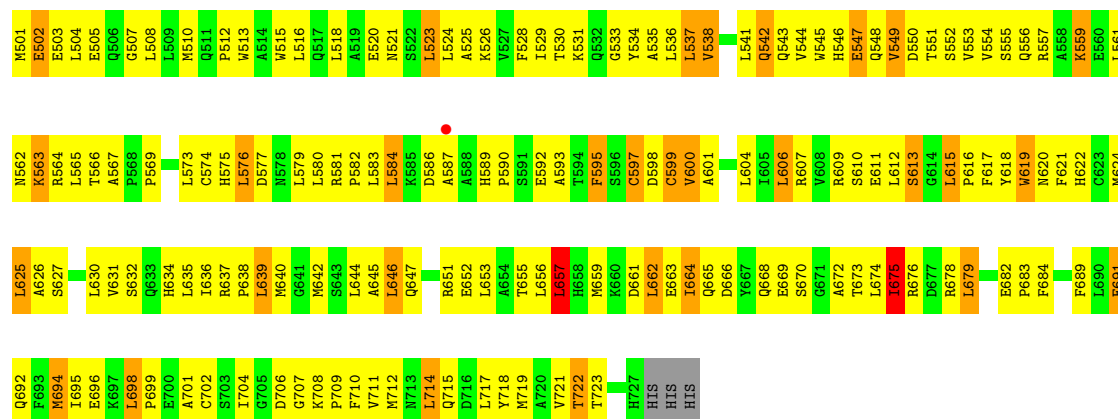
• Molecule 2: Non-homologous end-joining factor 1

Chain H: 26% 60% 12% .



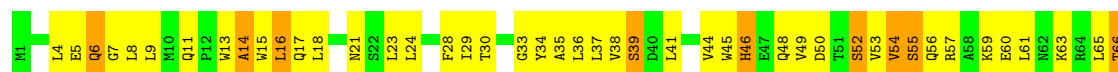
• Molecule 2: Non-homologous end-joining factor 1

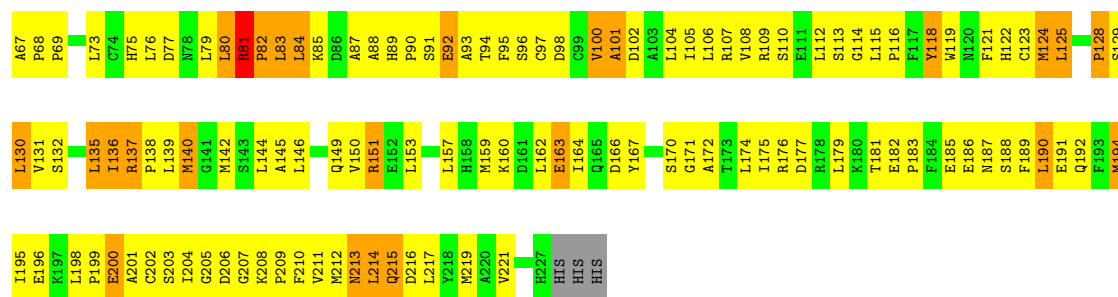
Chain I: 27% 58% 13% ..



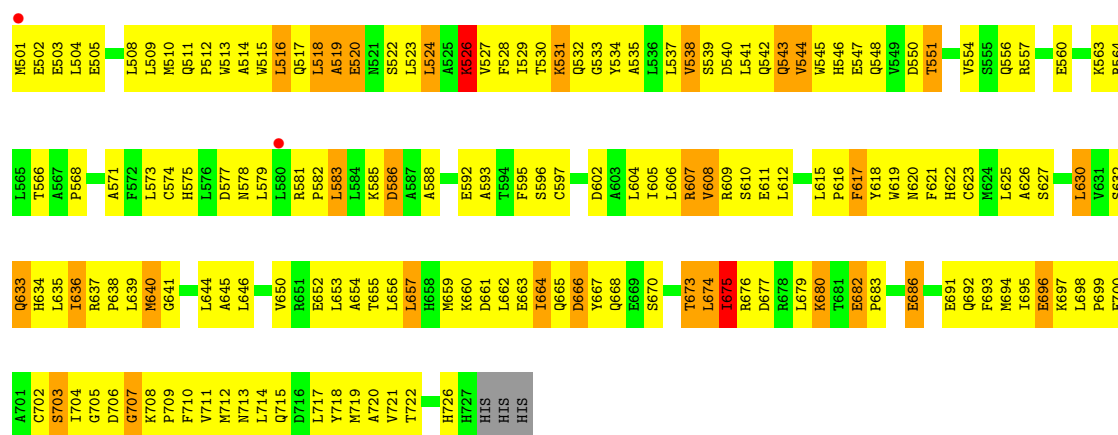
• Molecule 2: Non-homologous end-joining factor 1

Chain L: 27% 57% 14% .

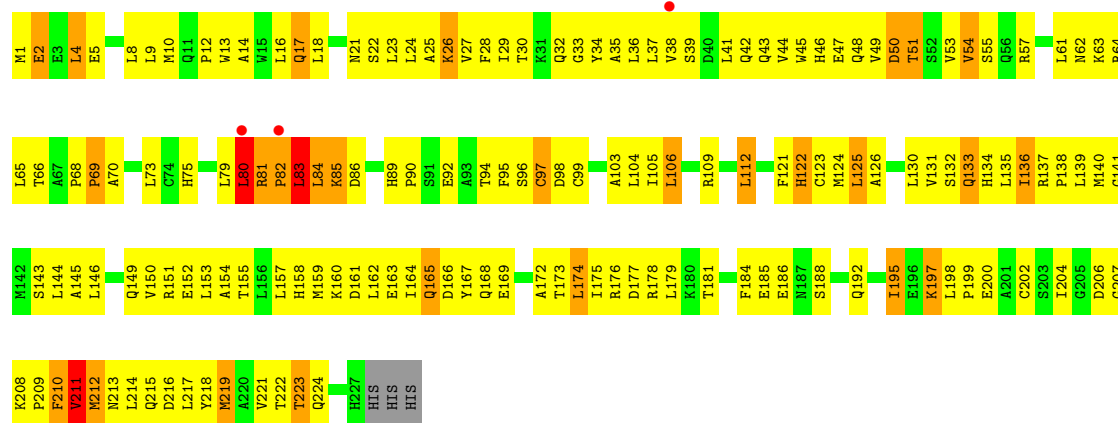




• Molecule 2: Non-homologous end-joining factor 1

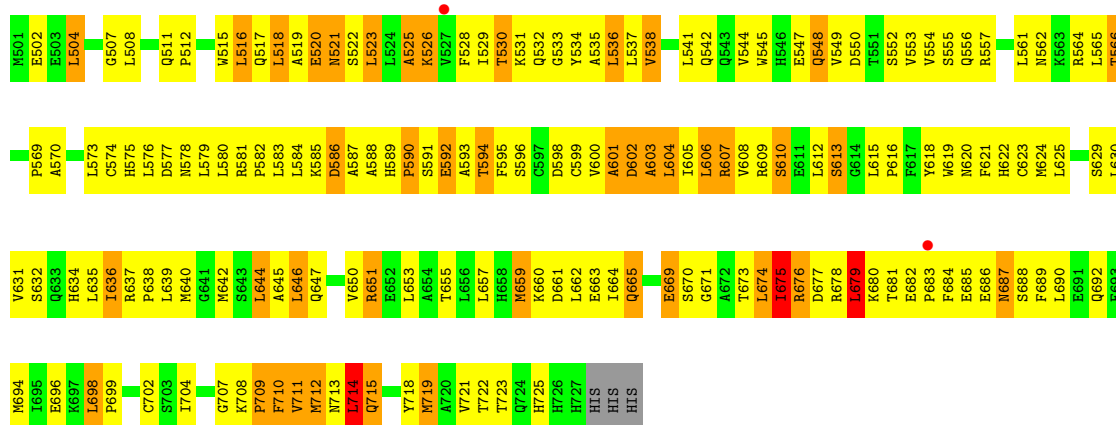


• Molecule 2: Non-homologous end-joining factor 1

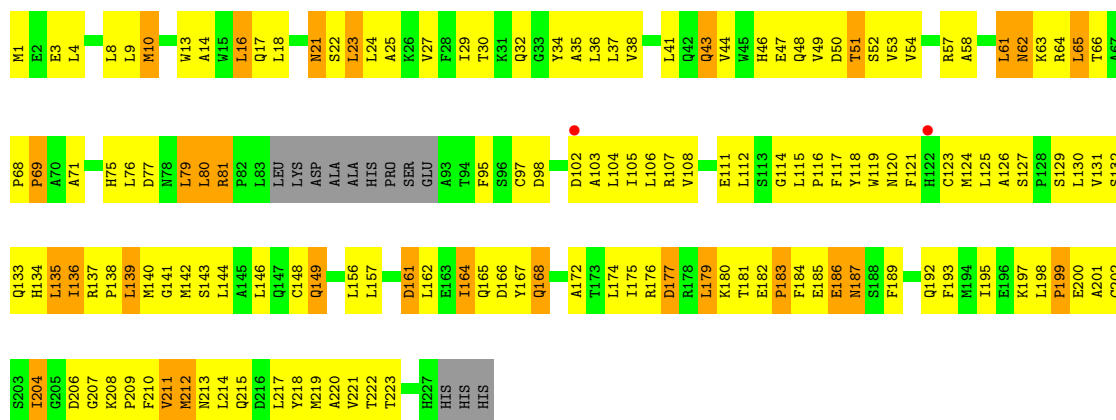


• Molecule 2: Non-homologous end-joining factor 1

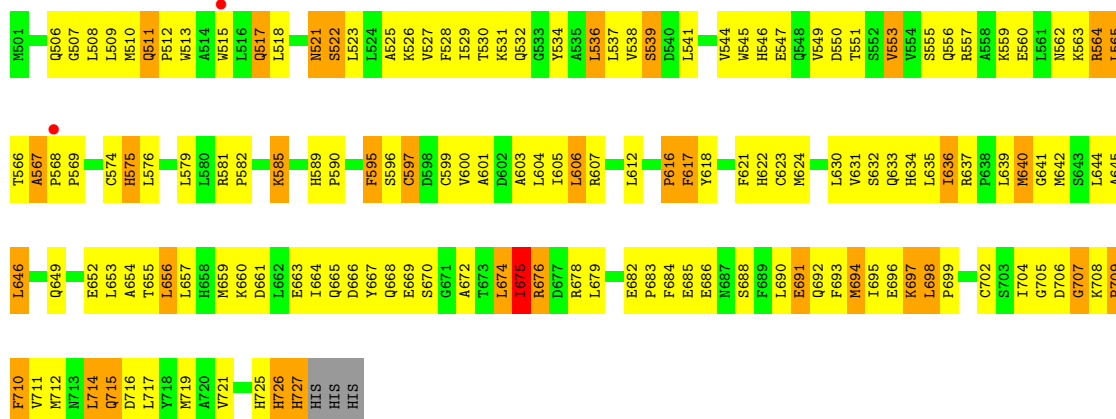




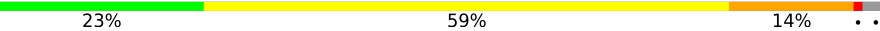
• Molecule 2: Non-homologous end-joining factor 1

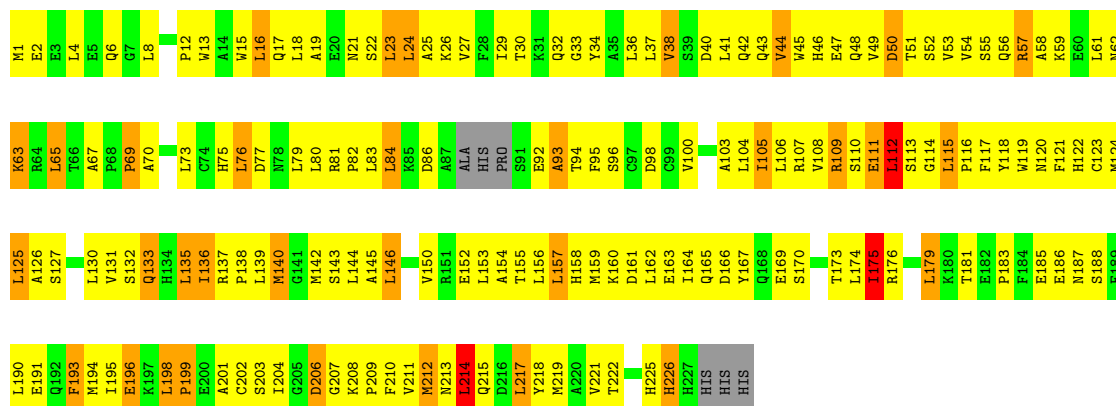


• Molecule 2: Non-homologous end-joining factor 1



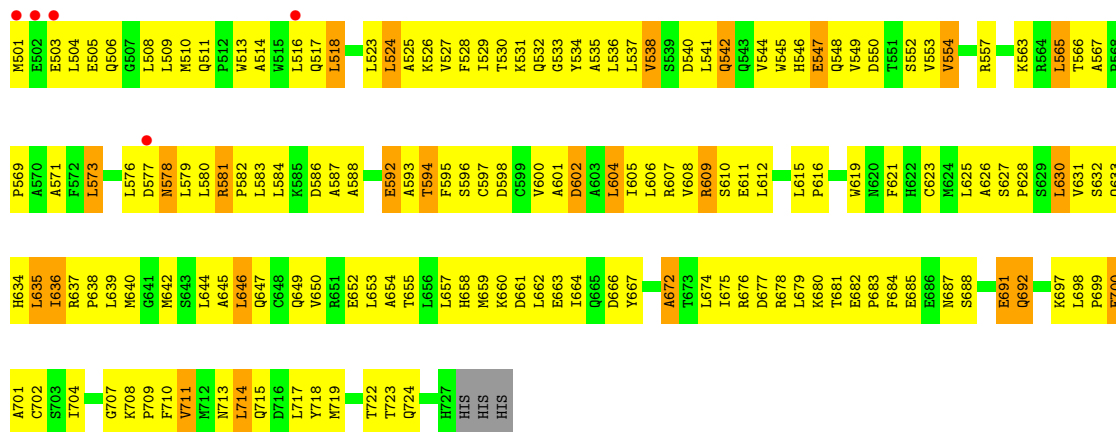
• Molecule 2: Non-homologous end-joining factor 1

Chain T:  23% 59% 14% ..



● Molecule 2: Non-homologous end-joining factor 1

Chain X:  2% 29% 59% 11% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	745.38Å 149.59Å 80.47Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	49.03 – 3.94 49.03 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.03-3.94) 99.2 (49.03-3.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.7.2_869, CNS	Depositor
R, R_{free}	0.271 , 0.326 0.241 , 0.304	Depositor DCC
R_{free} test set	3887 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	135.1	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 168.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	36833	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: TBR

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	0.27	0/1194	0.72	2/1608 (0.1%)
1	B	0.25	0/1262	0.74	1/1698 (0.1%)
1	F	0.26	0/1289	0.72	1/1737 (0.1%)
1	G	0.25	0/1289	0.70	1/1737 (0.1%)
1	J	0.26	0/1289	0.70	0/1737
1	K	0.26	0/1289	0.69	0/1737
1	N	0.27	0/1289	0.72	1/1737 (0.1%)
1	P	0.25	0/1289	0.73	0/1737
1	R	0.26	0/1289	0.73	0/1737
1	U	0.25	0/1289	0.68	0/1737
1	V	0.26	0/1289	0.70	0/1737
1	Y	0.25	0/1289	0.72	0/1737
2	D	0.27	0/1851	0.77	0/2511
2	E	0.27	0/1851	0.72	0/2511
2	H	0.27	0/1851	0.75	0/2511
2	I	0.27	0/1851	0.74	1/2511 (0.0%)
2	L	0.28	0/1851	0.75	2/2511 (0.1%)
2	M	0.26	0/1851	0.70	0/2511
2	O	0.27	0/1847	0.70	0/2507
2	Q	0.26	0/1851	0.76	2/2511 (0.1%)
2	S	0.27	0/1781	0.73	1/2414 (0.0%)
2	T	0.28	0/1826	0.73	1/2474 (0.0%)
2	W	0.29	0/1851	0.75	2/2511 (0.1%)
2	X	0.26	0/1851	0.75	2/2511 (0.1%)
All	All	0.27	0/37459	0.73	17/50670 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	711	VAL	N-CA-C	6.83	117.58	110.62
1	F	142	GLU	N-CA-C	-6.38	104.98	112.89
2	Q	602	ASP	CB-CA-C	-6.01	109.06	117.23
2	X	542	GLN	N-CA-C	-5.68	106.98	114.31
2	Q	519	ALA	CB-CA-C	-5.56	110.18	116.63

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	1171	0	1136	121	0
1	B	1239	0	1193	132	0
1	F	1264	0	1220	120	0
1	G	1264	0	1217	100	0
1	J	1264	0	1220	109	0
1	K	1264	0	1217	128	34
1	N	1264	0	1220	129	0
1	P	1264	0	1217	122	0
1	R	1264	0	1220	110	0
1	U	1264	0	1220	121	0
1	V	1264	0	1217	120	0
1	Y	1264	0	1217	99	0
2	D	1811	0	1811	236	0
2	E	1811	0	1808	260	0
2	H	1811	0	1811	225	0
2	I	1811	0	1808	229	0
2	L	1811	0	1811	231	0
2	M	1811	0	1808	241	0
2	O	1807	0	1800	181	0
2	Q	1811	0	1808	223	0
2	S	1744	0	1747	180	0
2	T	1789	0	1791	228	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	1811	0	1808	201	0
2	X	1811	0	1808	193	0
3	D	18	0	0	0	0
3	H	18	0	0	0	0
3	J	18	0	0	2	2
3	M	18	0	0	3	0
3	P	18	0	0	1	34
3	V	18	0	0	0	0
3	X	18	0	0	4	0
3	Y	18	0	0	3	0
All	All	36833	0	36133	3500	36

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 48.

The worst 5 of 3500 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)
2:X:605:ILE:CD1	3:X:5:TBR:BR4	2.35	1.28
2:M:560:GLU:OE2	3:M:164:TBR:BR8	2.13	1.22
2:X:605:ILE:HD13	3:X:5:TBR:BR4	1.99	1.14
1:A:18:HIS:HB3	1:A:36:LEU:HD11	1.29	1.13
2:E:606:LEU:HB2	2:E:621:PHE:HB2	1.31	1.11

The worst 5 of 36 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	Interatomic distance (Å)	Clash overlap (Å)
1:K:655:TRP:CB	3:P:2:TBR:BR9[1_554]	0.28	1.92
1:K:654:ASP:CA	3:P:2:TBR:TA6[1_554]	0.64	1.56
2:T:176:ARG:NH1	3:J:164:TBR:BR5[1_556]	0.77	1.43
1:K:654:ASP:CB	3:P:2:TBR:BRB[1_554]	1.19	1.01
1:K:654:ASP:C	3:P:2:TBR:TA6[1_554]	1.24	0.96

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	145/163 (89%)	108 (74%)	27 (19%)	10 (7%)	1	14
1	B	148/163 (91%)	116 (78%)	21 (14%)	11 (7%)	1	13
1	F	155/163 (95%)	120 (77%)	31 (20%)	4 (3%)	4	29
1	G	155/163 (95%)	114 (74%)	35 (23%)	6 (4%)	2	22
1	J	155/163 (95%)	114 (74%)	30 (19%)	11 (7%)	1	14
1	K	155/163 (95%)	110 (71%)	34 (22%)	11 (7%)	1	14
1	N	155/163 (95%)	121 (78%)	26 (17%)	8 (5%)	1	18
1	P	155/163 (95%)	126 (81%)	23 (15%)	6 (4%)	2	22
1	R	155/163 (95%)	125 (81%)	22 (14%)	8 (5%)	1	18
1	U	155/163 (95%)	130 (84%)	17 (11%)	8 (5%)	1	18
1	V	155/163 (95%)	126 (81%)	21 (14%)	8 (5%)	1	18
1	Y	155/163 (95%)	125 (81%)	20 (13%)	10 (6%)	1	15
2	D	225/230 (98%)	160 (71%)	51 (23%)	14 (6%)	1	16
2	E	225/230 (98%)	157 (70%)	50 (22%)	18 (8%)	1	12
2	H	225/230 (98%)	166 (74%)	45 (20%)	14 (6%)	1	16
2	I	225/230 (98%)	164 (73%)	52 (23%)	9 (4%)	2	21
2	L	225/230 (98%)	153 (68%)	56 (25%)	16 (7%)	1	14
2	M	225/230 (98%)	156 (69%)	51 (23%)	18 (8%)	1	12
2	O	225/230 (98%)	156 (69%)	51 (23%)	18 (8%)	1	12
2	Q	225/230 (98%)	156 (69%)	48 (21%)	21 (9%)	0	10
2	S	214/230 (93%)	151 (71%)	46 (22%)	17 (8%)	1	12
2	T	220/230 (96%)	161 (73%)	39 (18%)	20 (9%)	0	10
2	W	225/230 (98%)	169 (75%)	41 (18%)	15 (7%)	1	15
2	X	225/230 (98%)	156 (69%)	54 (24%)	15 (7%)	1	15
All	All	4527/4716 (96%)	3340 (74%)	891 (20%)	296 (6%)	1	15

5 of 296 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
2	D	94	THR
2	D	136	ILE
2	D	172	ALA
2	E	521	ASN

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	129/146 (88%)	109 (84%)	20 (16%)	2	15
1	B	138/146 (94%)	113 (82%)	25 (18%)	2	12
1	F	139/146 (95%)	119 (86%)	20 (14%)	3	17
1	G	139/146 (95%)	119 (86%)	20 (14%)	3	17
1	J	139/146 (95%)	127 (91%)	12 (9%)	10	33
1	K	139/146 (95%)	117 (84%)	22 (16%)	2	15
1	N	139/146 (95%)	120 (86%)	19 (14%)	3	17
1	P	139/146 (95%)	121 (87%)	18 (13%)	4	19
1	R	139/146 (95%)	130 (94%)	9 (6%)	15	42
1	U	139/146 (95%)	119 (86%)	20 (14%)	3	17
1	V	139/146 (95%)	115 (83%)	24 (17%)	2	12
1	Y	139/146 (95%)	118 (85%)	21 (15%)	3	16
2	D	201/204 (98%)	164 (82%)	37 (18%)	1	11
2	E	201/204 (98%)	166 (83%)	35 (17%)	2	12
2	H	201/204 (98%)	166 (83%)	35 (17%)	2	12
2	I	201/204 (98%)	171 (85%)	30 (15%)	3	16
2	L	201/204 (98%)	175 (87%)	26 (13%)	4	19
2	M	201/204 (98%)	177 (88%)	24 (12%)	5	21
2	O	200/204 (98%)	167 (84%)	33 (16%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	201/204 (98%)	166 (83%)	35 (17%)	2	12
2	S	194/204 (95%)	167 (86%)	27 (14%)	3	17
2	T	199/204 (98%)	167 (84%)	32 (16%)	2	14
2	W	201/204 (98%)	176 (88%)	25 (12%)	4	20
2	X	201/204 (98%)	178 (89%)	23 (11%)	5	22
All	All	4059/4200 (97%)	3467 (85%)	592 (15%)	3	16

5 of 592 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	164	ILE
1	Y	508	ILE
2	W	553	VAL
2	S	162	LEU
2	T	158	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	668	GLN
2	W	543	GLN
2	Q	727	HIS
1	V	637	ASN
2	T	17	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	X	5	-	0,36,36	-	-	-		
3	TBR	J	164	-	0,36,36	-	-	-		
3	TBR	Y	10	-	0,36,36	-	-	-		
3	TBR	D	231	-	0,36,36	-	-	-		
3	TBR	V	1	-	0,36,36	-	-	-		
3	TBR	M	164	-	0,36,36	-	-	-		
3	TBR	P	2	-	0,36,36	-	-	-		
3	TBR	H	231	-	0,36,36	-	-	-		

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.

5 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	5	TBR	4	0
3	J	164	TBR	2	2
3	Y	10	TBR	3	0
3	M	164	TBR	3	0
3	P	2	TBR	1	34

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	147/163 (90%)	-0.13	0 100 100	143, 217, 261, 290	0
1	B	152/163 (93%)	-0.12	1 (0%) 84 68	130, 199, 240, 289	0
1	F	157/163 (96%)	-0.19	1 (0%) 85 70	121, 173, 263, 314	0
1	G	157/163 (96%)	-0.21	1 (0%) 85 70	119, 173, 217, 265	0
1	J	157/163 (96%)	-0.08	4 (2%) 58 41	168, 209, 241, 255	0
1	K	157/163 (96%)	-0.24	0 100 100	175, 216, 268, 312	0
1	N	157/163 (96%)	-0.31	1 (0%) 85 70	115, 159, 206, 250	0
1	P	157/163 (96%)	-0.22	0 100 100	109, 169, 230, 262	0
1	R	157/163 (96%)	-0.35	1 (0%) 85 70	145, 184, 217, 234	0
1	U	157/163 (96%)	-0.33	0 100 100	147, 184, 233, 291	0
1	V	157/163 (96%)	-0.36	1 (0%) 85 70	123, 184, 219, 273	0
1	Y	157/163 (96%)	-0.26	1 (0%) 85 70	148, 202, 251, 276	0
2	D	227/230 (98%)	-0.15	1 (0%) 88 75	87, 144, 202, 244	0
2	E	227/230 (98%)	-0.20	0 100 100	99, 156, 233, 269	0
2	H	227/230 (98%)	-0.19	1 (0%) 88 75	107, 152, 210, 256	0
2	I	227/230 (98%)	-0.10	1 (0%) 88 75	113, 156, 213, 277	0
2	L	227/230 (98%)	-0.24	0 100 100	98, 152, 218, 251	0
2	M	227/230 (98%)	-0.21	2 (0%) 81 62	106, 167, 210, 244	0
2	O	227/230 (98%)	-0.15	3 (1%) 75 55	109, 165, 225, 311	0
2	Q	227/230 (98%)	-0.17	2 (0%) 81 62	99, 150, 211, 239	0
2	S	218/230 (94%)	-0.27	2 (0%) 81 62	111, 167, 216, 241	0
2	T	224/230 (97%)	-0.28	0 100 100	146, 199, 243, 267	0
2	W	227/230 (98%)	-0.20	2 (0%) 81 62	107, 160, 206, 242	0
2	X	227/230 (98%)	-0.18	5 (2%) 62 44	140, 189, 233, 303	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4581/4716 (97%)	-0.21	30 (0%) 84 68	87, 175, 238, 314	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	122	HIS	3.9
2	M	580	LEU	3.6
1	B	655	TRP	3.6
1	J	81	ALA	3.6
2	S	102	ASP	3.4

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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. 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	B-factors(Å ²)	Q<0.9
3	TBR	M	164	18/18	0.66	0.23	151,181,255,301	18
3	TBR	D	231	18/18	0.68	0.20	126,168,199,206	18
3	TBR	J	164	18/18	0.74	0.21	162,195,258,266	18
3	TBR	P	2	18/18	0.74	0.13	210,281,466,490	18
3	TBR	Y	10	18/18	0.82	0.12	130,168,192,193	18
3	TBR	H	231	18/18	0.83	0.18	128,160,180,224	18
3	TBR	X	5	18/18	0.84	0.14	134,172,195,230	18
3	TBR	V	1	18/18	0.84	0.14	103,151,191,204	18

6.5 Other polymers ⓘ

There are no such residues in this entry.