



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:02 AM GMT

PDB ID : 3D1N  
Title : Structure of human Brn-5 transcription factor in complex with corticotrophin  
-releasing hormone gene promoter  
Authors : Pereira, J.H.; Ha, S.C.; Kim, S.-H.  
Deposited on : 2008-05-06  
Resolution : 2.51 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](mailto: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.

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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

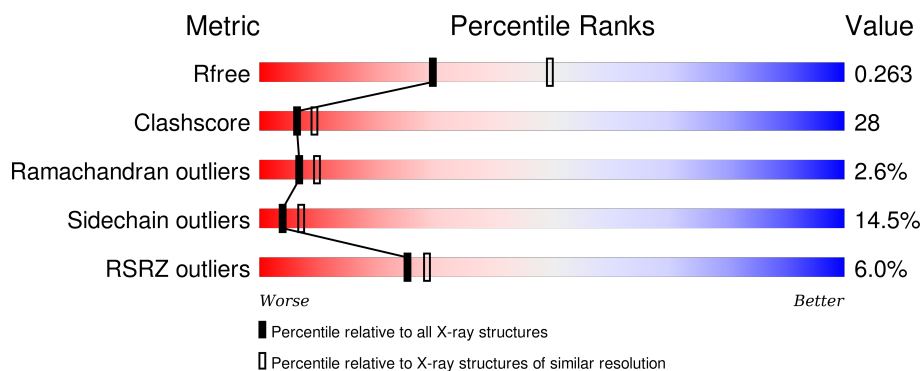
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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.





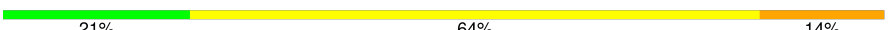

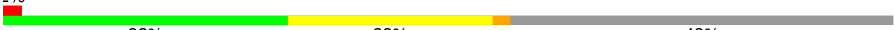
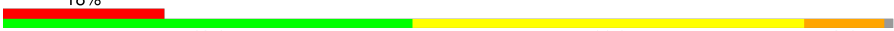




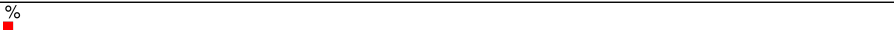
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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	14	
1	C	14	
1	E	14	
1	G	14	
2	B	14	

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Mol	Chain	Length	Quality of chain
2	D	14	 50% 50%
2	F	14	 50% 50%
2	H	14	 21% 64% 14%
3	I	151	 50% 37% 13% •
3	J	151	 2% 32% 23% • 43%
3	K	151	 18% 46% 44% 9% •
3	L	151	 8% 57% 32% 7% •
3	M	151	 2% 48% 38% 14% •
3	N	151	 3% 30% 22% • 44%
3	O	151	 9% 46% 45% 8% ••
3	P	151	 % 36% 16% • 46%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10089 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 DNA chain called 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	C	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	E	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	G	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			

- Molecule 2 is a DNA chain called 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	D	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	F	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	H	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			

- Molecule 3 is a protein called POU domain, class 6, transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	150	Total	C	N	O	Se	0	0	0
			1192	746	216	226	4			
3	J	86	Total	C	N	O	Se	0	0	0
			666	420	114	129	3			
3	K	150	Total	C	N	O	Se	0	0	0
			1100	689	194	213	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	145	Total	C	N	O	Se	0	0	0
			1130	708	203	215	4			
3	M	150	Total	C	N	O	Se	0	0	0
			1188	742	215	227	4			
3	N	85	Total	C	N	O	Se	0	0	0
			658	414	113	128	3			
3	O	150	Total	C	N	O	Se	0	0	0
			1166	730	209	223	4			
3	P	82	Total	C	N	O	Se	0	0	0
			620	390	108	119	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	144	MSE	LEU	ENGINEERED	UNP Q14863
I	172	MSE	LEU	ENGINEERED	UNP Q14863
I	186	SER	CYS	ENGINEERED	UNP Q14863
I	267	MSE	ILE	ENGINEERED	UNP Q14863
I	283	SER	CYS	ENGINEERED	UNP Q14863
J	144	MSE	LEU	ENGINEERED	UNP Q14863
J	172	MSE	LEU	ENGINEERED	UNP Q14863
J	186	SER	CYS	ENGINEERED	UNP Q14863
J	267	MSE	ILE	ENGINEERED	UNP Q14863
J	283	SER	CYS	ENGINEERED	UNP Q14863
K	144	MSE	LEU	ENGINEERED	UNP Q14863
K	172	MSE	LEU	ENGINEERED	UNP Q14863
K	186	SER	CYS	ENGINEERED	UNP Q14863
K	267	MSE	ILE	ENGINEERED	UNP Q14863
K	283	SER	CYS	ENGINEERED	UNP Q14863
L	144	MSE	LEU	ENGINEERED	UNP Q14863
L	172	MSE	LEU	ENGINEERED	UNP Q14863
L	186	SER	CYS	ENGINEERED	UNP Q14863
L	267	MSE	ILE	ENGINEERED	UNP Q14863
L	283	SER	CYS	ENGINEERED	UNP Q14863
M	144	MSE	LEU	ENGINEERED	UNP Q14863
M	172	MSE	LEU	ENGINEERED	UNP Q14863
M	186	SER	CYS	ENGINEERED	UNP Q14863
M	267	MSE	ILE	ENGINEERED	UNP Q14863
M	283	SER	CYS	ENGINEERED	UNP Q14863
N	144	MSE	LEU	ENGINEERED	UNP Q14863
N	172	MSE	LEU	ENGINEERED	UNP Q14863
N	186	SER	CYS	ENGINEERED	UNP Q14863
N	267	MSE	ILE	ENGINEERED	UNP Q14863

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Chain	Residue	Modelled	Actual	Comment	Reference
N	283	SER	CYS	ENGINEERED	UNP Q14863
O	144	MSE	LEU	ENGINEERED	UNP Q14863
O	172	MSE	LEU	ENGINEERED	UNP Q14863
O	186	SER	CYS	ENGINEERED	UNP Q14863
O	267	MSE	ILE	ENGINEERED	UNP Q14863
O	283	SER	CYS	ENGINEERED	UNP Q14863
P	144	MSE	LEU	ENGINEERED	UNP Q14863
P	172	MSE	LEU	ENGINEERED	UNP Q14863
P	186	SER	CYS	ENGINEERED	UNP Q14863
P	267	MSE	ILE	ENGINEERED	UNP Q14863
P	283	SER	CYS	ENGINEERED	UNP Q14863

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	10	Total O 10 10	0	0
4	C	5	Total O 5 5	0	0
4	D	1	Total O 1 1	0	0
4	E	9	Total O 9 9	0	0
4	F	10	Total O 10 10	0	0
4	G	4	Total O 4 4	0	0
4	H	5	Total O 5 5	0	0
4	I	8	Total O 8 8	0	0
4	J	6	Total O 6 6	0	0
4	L	1	Total O 1 1	0	0
4	M	10	Total O 10 10	0	0
4	N	6	Total O 6 6	0	0
4	O	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	3	Total	O	0	0
			3	3		

### 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 ( $RSRZ > 2$ ). 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.

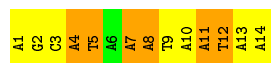
- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain A: 



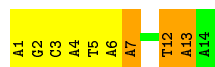
- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain C: 




- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain E: 



- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain G: 



- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'

Chain B: 






- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'

Chain D: 

T1 T2 A3 T4 T5 A6 T7 T8 T9 A10 A11 T11 G12 C13 T14

- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'

Chain F: 

T1 T2 A3 T4 T5 A6 T7 T8 T9 A10 A11 T11 G12 C13 T14

- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'

Chain H: 

T1 T2 A3 T4 T5 A6 T7 T8 T9 A10 G13 T14


- Molecule 3: POU domain, class 6, transcription factor 1

Chain I: 

I1E M143 M144 M145 E146 E147 I148 E149 F150 R157 R158 L161 T166 Q167 V168 G169 Q170 A171 M172 T173 A179 Y180 S181 I185 K190 L191 T194 P195 K196 S197 A198 Q199 K202 P203 V204 L205 E206 L209 E213 L214 R215 E218 G219 Q220 Q221 N222 L223 M224 E225

F226 G229 E230 P231 S232 K236 R237 R238 T239 E247 A248 L249 M250 A251 V252 F253 E254 K255 L258 P259 T260 Q262 E263 L264 T265 E266 M267 A268 K269 E276 R279 N284 R285 R286 Q287 T288 L289 N291 T292

- Molecule 3: POU domain, class 6, transcription factor 1

Chain J: 

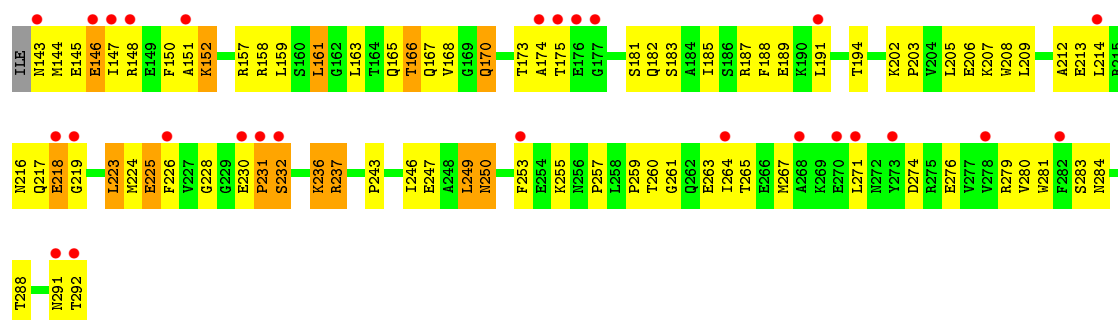
I142 M143 M144 E145 E146 I147 R148 E149 R157 L161 G162 L163 T164 Q165 T166 Q167 V168 G169 Q170 A171 M172 T175 E176 G177 P178 A179 Y180 S181 Q182 S183 A184 I185 S186 R187 K190 L191 D192 K200 L201 K202 P203 V204 L205 L209 A212 R215 R218 E218 N222 L223 M224

E225 F226 G227 G228 G229 G230 G231 G232 G233 G234 G235 G236 G237 G238 G239 G240 G241 G242 G243 G244 G245 G246 G247 G248 G249 G250 G251 G252 G253 G254 G255 G256 G257 G258 G259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279 G280 G281 G282 G283 G284 G285 G286 G287 G288 G289 G290 G291 G292 G293 G294 G295 G296 G297 G298 G299 G300 G301 G302 G303 G304 G305 G306 G307 G308 G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 G325 G326 G327 G328 G329 G330 G331 G332 G333 G334 G335 G336 G337 G338 G339 G340 G341 G342 G343 G344 G345 G346 G347 G348 G349 G350 G351 G352 G353 G354 G355 G356 G357 G358 G359 G360 G361 G362 G363 G364 G365 G366 G367 G368 G369 G370 G371 G372 G373 G374 G375 G376 G377 G378 G379 G380 G381 G382 G383 G384 G385 G386 G387 G388 G389 G390 G391 G392 G393 G394 G395 G396 G397 G398 G399 G400 G401 G402 G403 G404 G405 G406 G407 G408 G409 G410 G411 G412 G413 G414 G415 G416 G417 G418 G419 G420 G421 G422 G423 G424 G425 G426 G427 G428 G429 G430 G431 G432 G433 G434 G435 G436 G437 G438 G439 G440 G441 G442 G443 G444 G445 G446 G447 G448 G449 G450 G451 G452 G453 G454 G455 G456 G457 G458 G459 G460 G461 G462 G463 G464 G465 G466 G467 G468 G469 G470 G471 G472 G473 G474 G475 G476 G477 G478 G479 G480 G481 G482 G483 G484 G485 G486 G487 G488 G489 G490 G491 G492 G493 G494 G495 G496 G497 G498 G499 G500 G501 G502 G503 G504 G505 G506 G507 G508 G509 G510 G511 G512 G513 G514 G515 G516 G517 G518 G519 G520 G521 G522 G523 G524 G525 G526 G527 G528 G529 G530 G531 G532 G533 G534 G535 G536 G537 G538 G539 G540 G541 G542 G543 G544 G545 G546 G547 G548 G549 G550 G551 G552 G553 G554 G555 G556 G557 G558 G559 G560 G561 G562 G563 G564 G565 G566 G567 G568 G569 G570 G571 G572 G573 G574 G575 G576 G577 G578 G579 G580 G581 G582 G583 G584 G585 G586 G587 G588 G589 G590 G591 G592 G593 G594 G595 G596 G597 G598 G599 G600 G601 G602 G603 G604 G605 G606 G607 G608 G609 G610 G611 G612 G613 G614 G615 G616 G617 G618 G619 G620 G621 G622 G623 G624 G625 G626 G627 G628 G629 G630 G631 G632 G633 G634 G635 G636 G637 G638 G639 G640 G641 G642 G643 G644 G645 G646 G647 G648 G649 G650 G651 G652 G653 G654 G655 G656 G657 G658 G659 G660 G661 G662 G663 G664 G665 G666 G667 G668 G669 G670 G671 G672 G673 G674 G675 G676 G677 G678 G679 G680 G681 G682 G683 G684 G685 G686 G687 G688 G689 G690 G691 G692 G693 G694 G695 G696 G697 G698 G699 G700 G701 G702 G703 G704 G705 G706 G707 G708 G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 G725 G726 G727 G728 G729 G730 G731 G732 G733 G734 G735 G736 G737 G738 G739 G740 G741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 G753 G754 G755 G756 G757 G758 G759 G760 G761 G762 G763 G764 G765 G766 G767 G768 G769 G770 G771 G772 G773 G774 G775 G776 G777 G778 G779 G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G792 G793 G794 G795 G796 G797 G798 G799 G800 G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860 G861 G862 G863 G864 G865 G866 G867 G868 G869 G870 G871 G872 G873 G874 G875 G876 G877 G878 G879 G880 G881 G882 G883 G884 G885 G886 G887 G888 G889 G890 G891 G892 G893 G894 G895 G896 G897 G898 G899 G900 G901 G902 G903 G904 G905 G906 G907 G908 G909 G910 G911 G912 G913 G914 G915 G916 G917 G918 G919 G920 G921 G922 G923 G924 G925 G926 G927 G928 G929 G930 G931 G932 G933 G934 G935 G936 G937 G938 G939 G940 G941 G942 G943 G944 G945 G946 G947 G948 G949 G950 G951 G952 G953 G954 G955 G956 G957 G958 G959 G960 G961 G962 G963 G964 G965 G966 G967 G968 G969 G970 G971 G972 G973 G974 G975 G976 G977 G978 G979 G980 G981 G982 G983 G984 G985 G986 G987 G988 G989 G990 G991 G992 G993 G994 G995 G996 G997 G998 G999

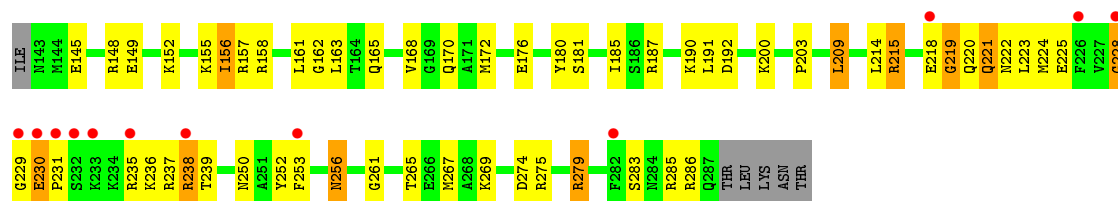
ARG ARG GLN THR LEU LEU ASN THR

- Molecule 3: POU domain, class 6, transcription factor 1

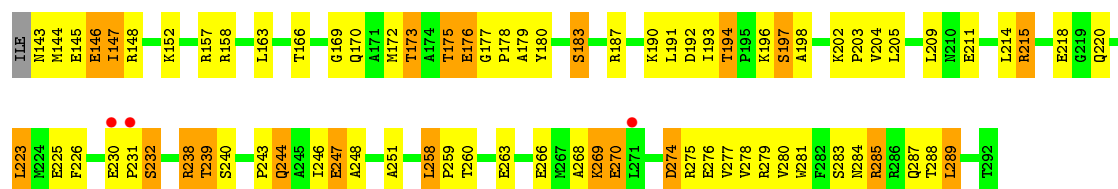
Chain K: 



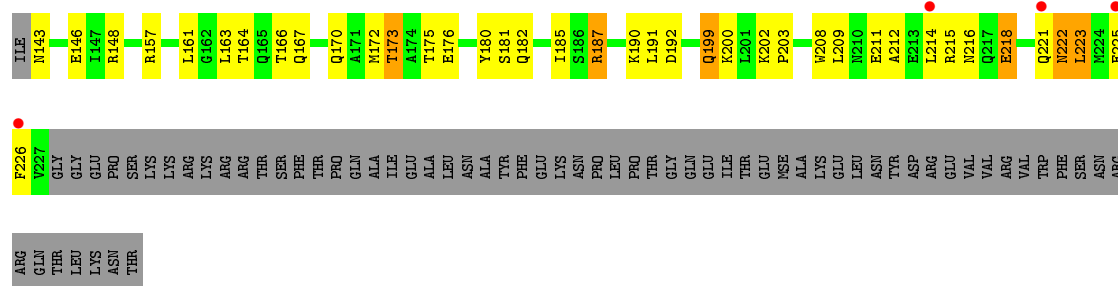
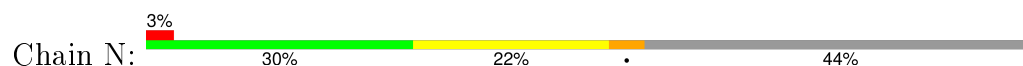
- Molecule 3: POU domain, class 6, transcription factor 1



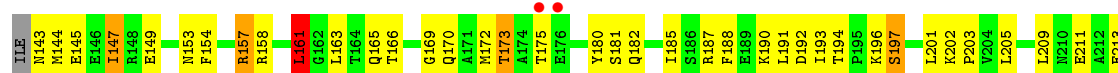
- Molecule 3: POU domain, class 6, transcription factor 1

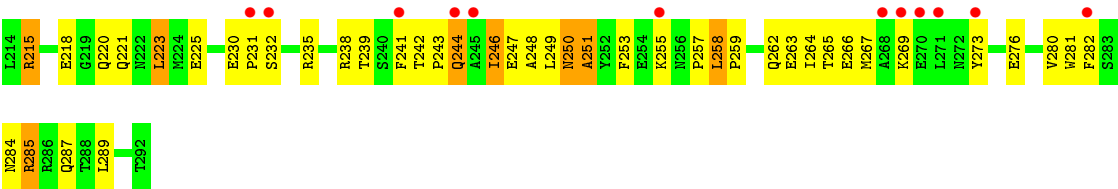


- Molecule 3: POU domain, class 6, transcription factor 1

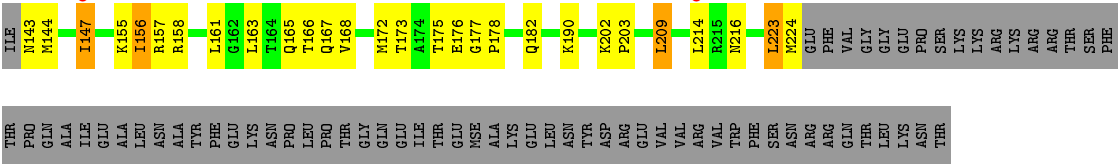
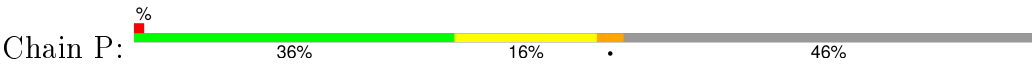


- Molecule 3: POU domain, class 6, transcription factor 1





● Molecule 3: POU domain, class 6, transcription factor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.30Å 112.06Å 181.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.51 48.91 – 2.51	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.91-2.51) 74.7 (48.91-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	65.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.270 0.205 , 0.263	Depositor DCC
$R_{free}$ test set	2672 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 76.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 52734 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [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	0.80	0/324	1.84	11/498 (2.2%)
1	C	0.79	0/324	1.89	13/498 (2.6%)
1	E	0.95	0/324	1.93	13/498 (2.6%)
1	G	0.87	0/324	1.89	12/498 (2.4%)
2	B	0.83	0/312	1.95	13/480 (2.7%)
2	D	0.85	0/312	2.17	15/480 (3.1%)
2	F	0.85	0/312	2.19	21/480 (4.4%)
2	H	0.96	0/312	2.03	10/480 (2.1%)
3	I	0.42	0/1208	0.59	0/1622
3	J	0.41	0/672	0.57	0/900
3	K	0.29	0/1114	0.52	0/1507
3	L	0.36	0/1146	0.55	0/1540
3	M	0.42	0/1204	0.65	0/1620
3	N	0.41	0/664	0.60	0/889
3	O	0.36	0/1182	0.55	0/1593
3	P	0.38	0/625	0.55	0/836
All	All	0.54	0/10359	1.15	108/14419 (0.7%)

There are no bond length outliers.

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	DT	O4'-C1'-N1	-13.05	98.87	108.00
2	D	9	DT	O4'-C1'-N1	13.04	117.13	108.00
2	D	12	DG	O4'-C1'-N9	-11.20	100.16	108.00
2	D	5	DT	O4'-C1'-N1	-10.91	100.36	108.00
1	A	5	DT	O4'-C1'-N1	10.16	115.11	108.00

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	287	0	159	13	0
1	C	287	0	159	7	0
1	E	287	0	159	8	0
1	G	287	0	159	8	0
2	B	281	0	165	14	0
2	D	281	0	165	18	0
2	F	281	0	165	21	0
2	H	281	0	165	11	0
3	I	1192	0	1174	65	0
3	J	666	0	654	28	0
3	K	1100	0	1017	68	0
3	L	1130	0	1090	62	0
3	M	1188	0	1157	81	0
3	N	658	0	643	39	0
3	O	1166	0	1120	80	0
3	P	620	0	606	22	0
4	A	9	0	0	5	0
4	B	10	0	0	2	0
4	C	5	0	0	0	0
4	D	1	0	0	0	0
4	E	9	0	0	2	0
4	F	10	0	0	3	0
4	G	4	0	0	0	0
4	H	5	0	0	0	0
4	I	8	0	0	2	0
4	J	6	0	0	1	0
4	L	1	0	0	0	0
4	M	10	0	0	1	0
4	N	6	0	0	2	0
4	O	10	0	0	0	0
4	P	3	0	0	1	0
All	All	10089	0	8757	512	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 28.

The worst 5 of 512 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)
3:L:265:THR:HG22	3:L:275:ARG:HE	1.09	1.15
3:L:238:ARG:HG2	3:L:238:ARG:HH11	1.03	1.15
3:M:238:ARG:HH11	3:M:238:ARG:HG2	1.18	1.06
3:K:250:ASN:HA	3:K:253:PHE:HB3	1.38	1.03
2:F:9:DT:OP2	3:N:166:THR:HG23	1.59	1.03

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	
3	I	148/151 (98%)	123 (83%)	17 (12%)	8 (5%)	2	2
3	J	84/151 (56%)	78 (93%)	6 (7%)	0	100	100
3	K	148/151 (98%)	119 (80%)	22 (15%)	7 (5%)	3	3
3	L	143/151 (95%)	122 (85%)	16 (11%)	5 (4%)	4	6
3	M	148/151 (98%)	136 (92%)	10 (7%)	2 (1%)	14	24
3	N	83/151 (55%)	79 (95%)	3 (4%)	1 (1%)	16	29
3	O	148/151 (98%)	127 (86%)	19 (13%)	2 (1%)	14	24
3	P	80/151 (53%)	70 (88%)	9 (11%)	1 (1%)	15	26
All	All	982/1208 (81%)	854 (87%)	102 (10%)	26 (3%)	7	10

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	230	GLU
3	I	231	PRO
3	I	232	SER
3	K	218	GLU
3	N	218	GLU

### 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	
3	I	125/129 (97%)	103 (82%)	22 (18%)	2	4
3	J	69/129 (54%)	63 (91%)	6 (9%)	13	24
3	K	105/129 (81%)	89 (85%)	16 (15%)	3	6
3	L	115/129 (89%)	105 (91%)	10 (9%)	13	24
3	M	124/129 (96%)	96 (77%)	28 (23%)	1	1
3	N	68/129 (53%)	63 (93%)	5 (7%)	17	31
3	O	119/129 (92%)	98 (82%)	21 (18%)	2	4
3	P	62/129 (48%)	56 (90%)	6 (10%)	10	19
All	All	787/1032 (76%)	673 (86%)	114 (14%)	4	7

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	279	ARG
3	M	197	SER
3	O	269	LYS
3	L	286	ARG
3	M	170	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	287	GLN
3	N	199	GLN
3	P	199	GLN
3	N	170	GLN
3	N	216	ASN

### 5.3.3 RNA ⓘ

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](#)

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	14/14 (100%)	0.10	0 100 100	36, 43, 52, 53	0
1	C	14/14 (100%)	-0.11	0 100 100	42, 48, 57, 58	0
1	E	14/14 (100%)	0.00	0 100 100	33, 37, 49, 53	0
1	G	14/14 (100%)	-0.05	0 100 100	35, 41, 59, 59	0
2	B	14/14 (100%)	-0.04	0 100 100	34, 46, 58, 59	0
2	D	14/14 (100%)	-0.13	0 100 100	43, 50, 54, 55	0
2	F	14/14 (100%)	0.02	0 100 100	33, 41, 45, 55	0
2	H	14/14 (100%)	-0.10	0 100 100	37, 44, 48, 52	0
3	I	146/151 (96%)	-0.02	0 100 100	34, 67, 102, 131	0
3	J	83/151 (54%)	0.18	3 (3%) 46 51	37, 60, 91, 103	0
3	K	146/151 (96%)	1.08	27 (18%) 2 2	51, 107, 136, 146	0
3	L	141/151 (93%)	0.49	12 (8%) 13 14	46, 67, 114, 142	0
3	M	146/151 (96%)	0.02	3 (2%) 67 71	33, 57, 91, 123	0
3	N	82/151 (54%)	0.27	4 (4%) 33 38	38, 58, 88, 106	0
3	O	146/151 (96%)	0.43	14 (9%) 10 11	40, 79, 122, 136	0
3	P	79/151 (52%)	0.14	2 (2%) 61 65	43, 73, 107, 119	0
All	All	1081/1320 (81%)	0.31	65 (6%) 25 28	33, 67, 121, 146	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	175	THR	8.9
3	K	292	THR	8.2
3	K	174	ALA	7.6
3	L	231	PRO	5.7
3	O	268	ALA	5.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.