wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:54 PM GMT

PDB ID	:	1HMV
Title	:	THE STRUCTURE OF UNLIGANDED REVERSE TRANSCRIPTASE FROM THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors	:	Rodgers, D.W.; Gamblin, S.J.; Harris, B.A.; Ray, S.; Culp, J.S.; Hellmig, B.; Woolf, D.J.; Debouck, C.; Harrison, S.C.
Deposited on	:	1994-12-15
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
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:

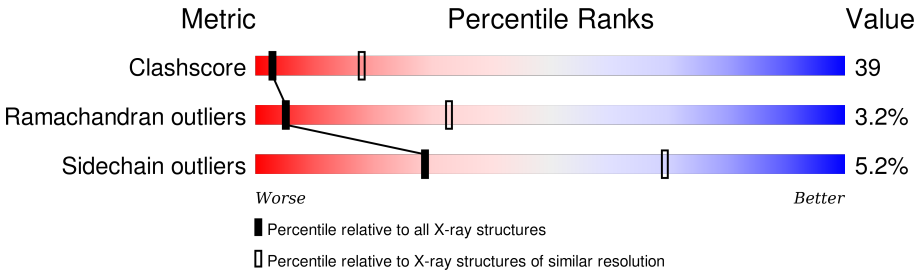
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	40% 51%
1	C	560	39% 52%
1	E	560	40% 51%
1	G	560	39% 52%
2	B	440	39% 45% 10%
2	D	440	40% 45% 10%
2	F	440	40% 45% 10%

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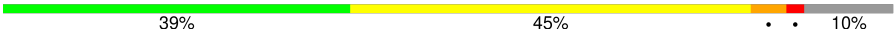
Mol	Chain	Length	Quality of chain
2	H	440	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29596 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 HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	C	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	E	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	G	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	D	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	F	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	H	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

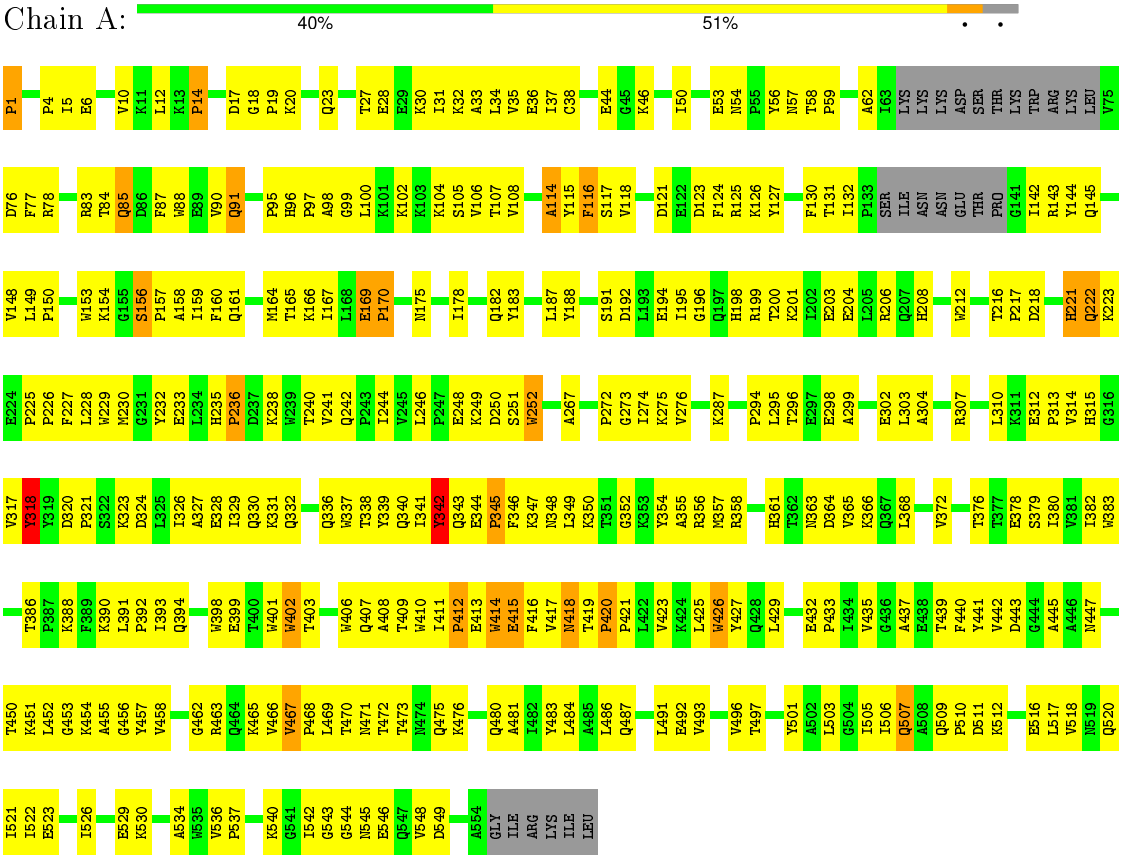
3 Residue-property plots (i)

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.

Note EDS was not executed.

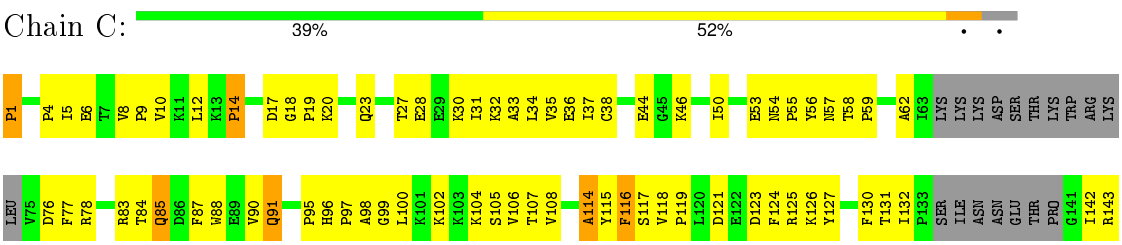
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

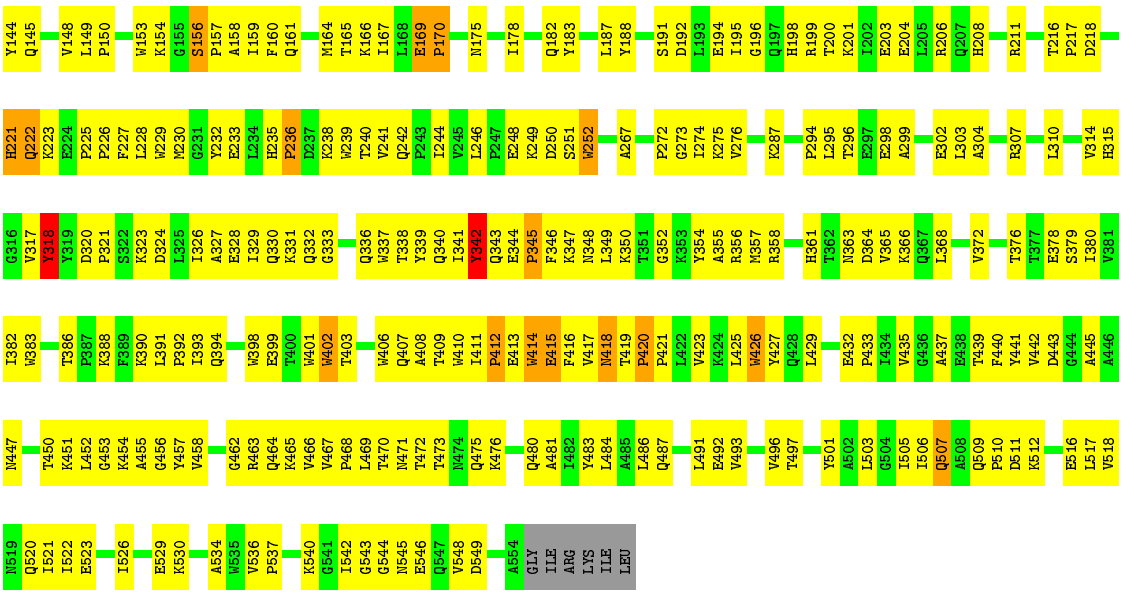
Chain A:



- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

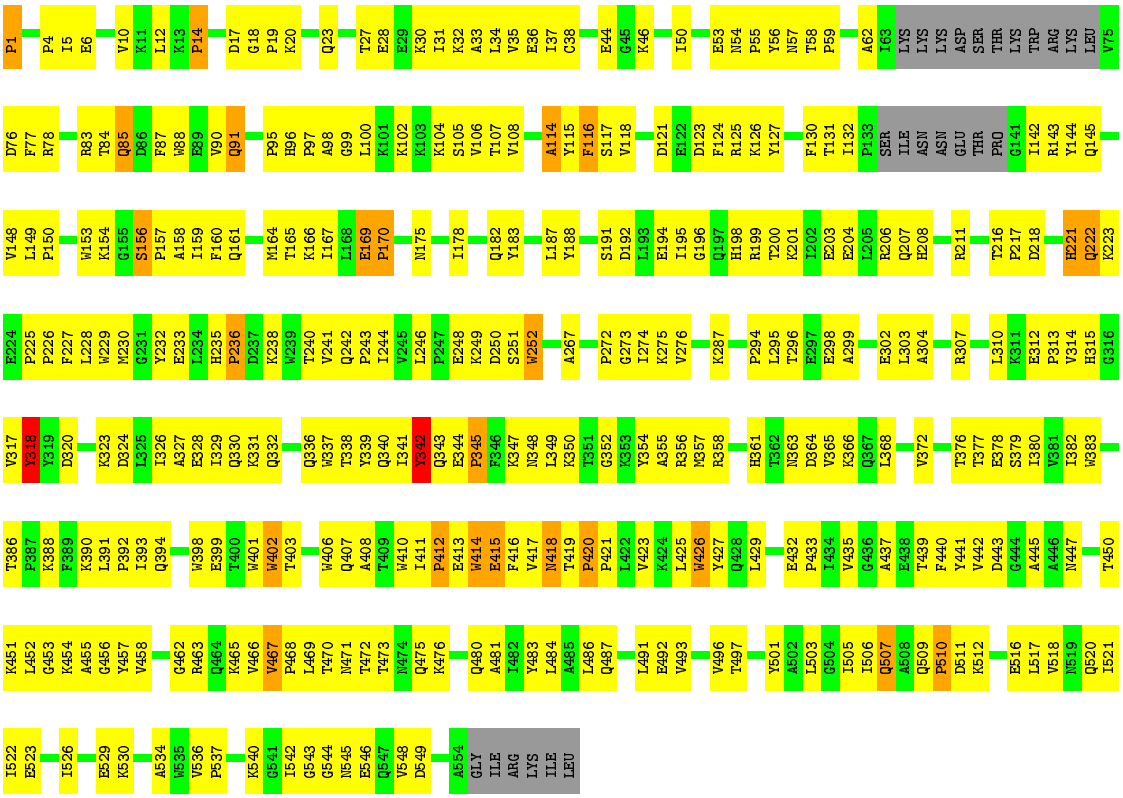
Chain C:





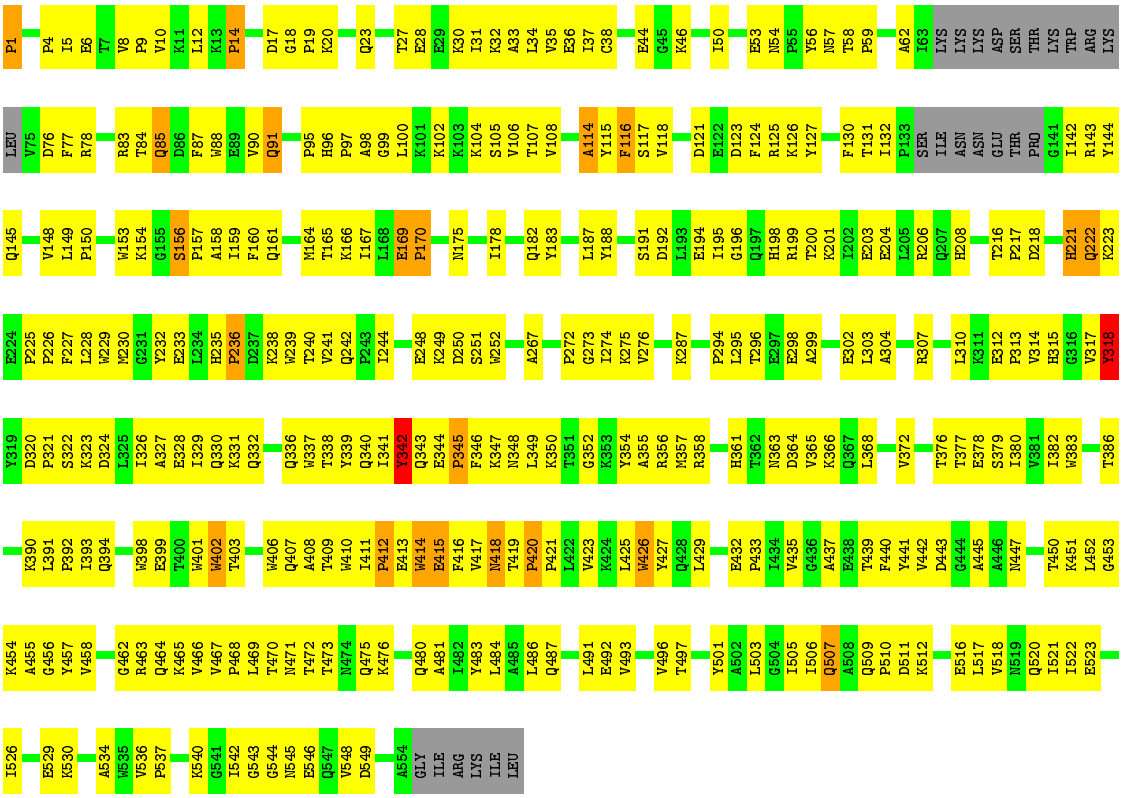
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

Chain E:



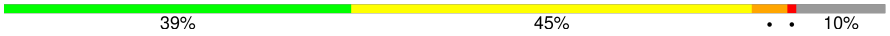
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

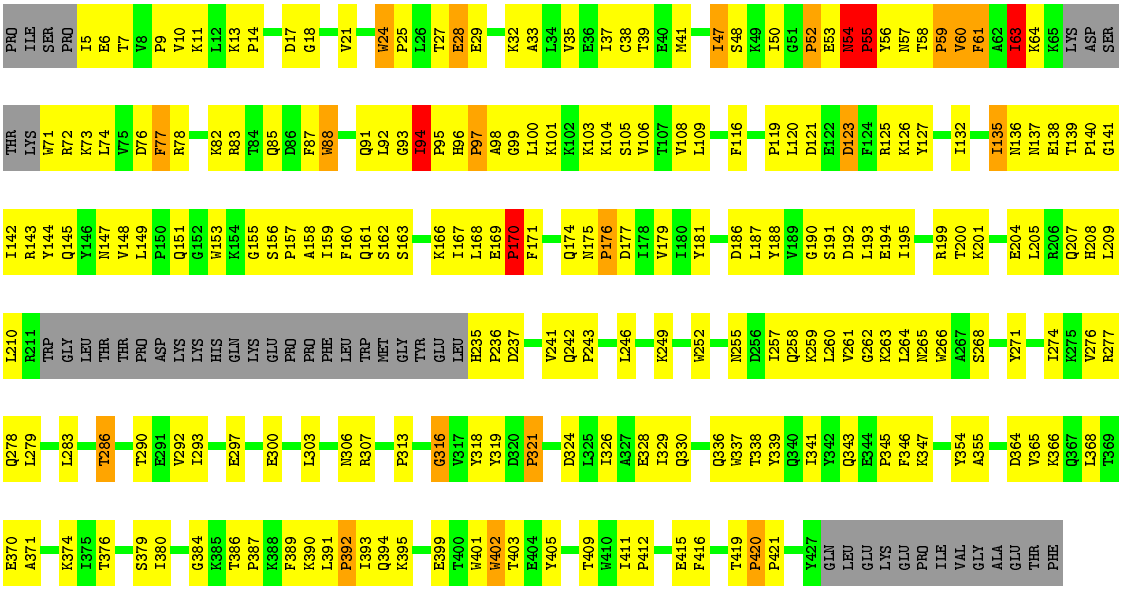
Chain G:



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

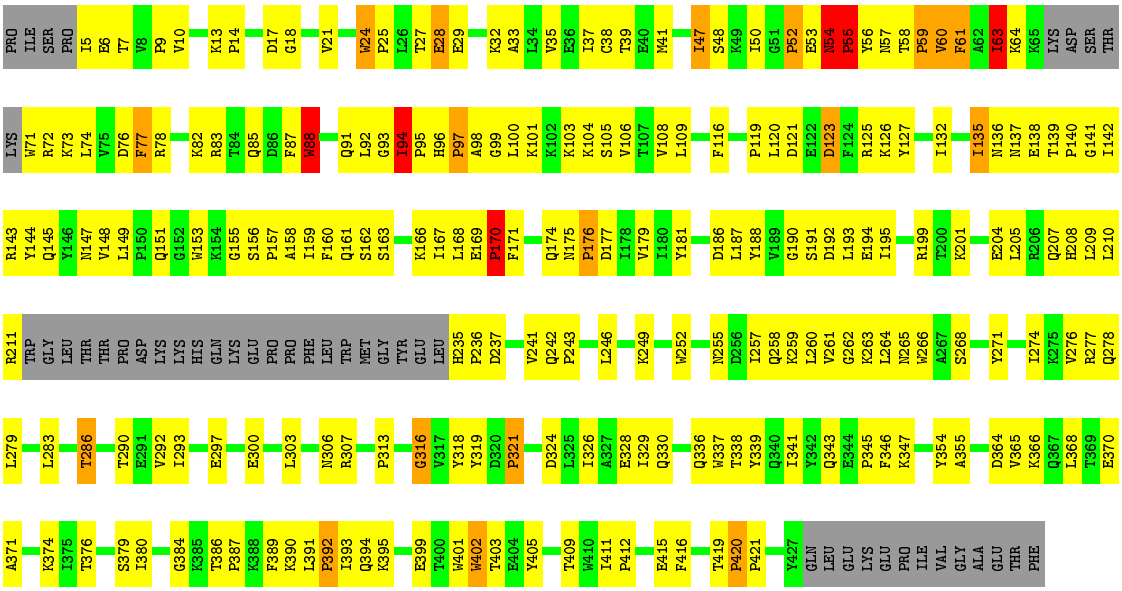
Chain B:





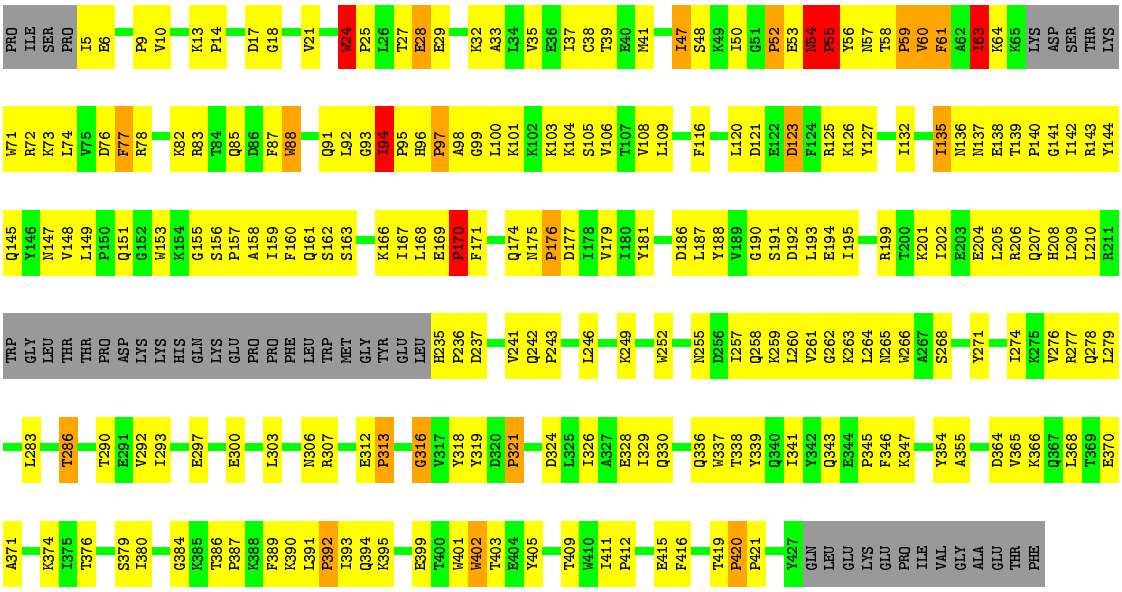
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain D:



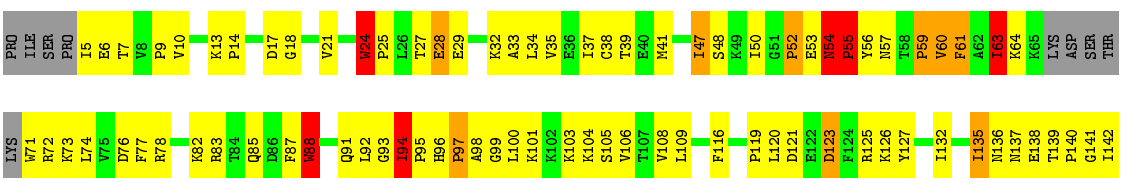
- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

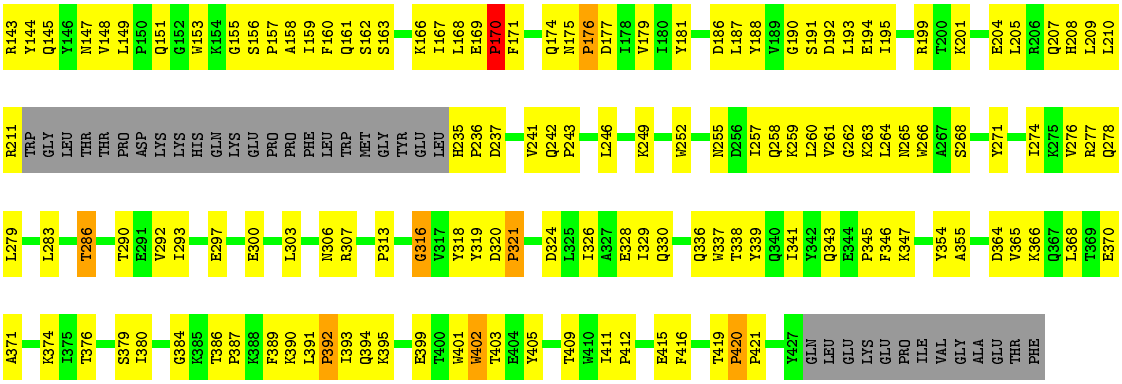
Chain F:



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain H:




R143 Y144 Q145 Y146 N147 V148 L149 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159 F160 Q161 S162 S163 K166 I167 L168 E169 P170 F171 Q174 N175 P176 D177 I178 V179 I180 Y181 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195 R199 T200 K201 E204 L205 R206 Q207 H208 L209 L210
R211 TRP GLY LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY TYR GLU LEU H235 P236 D237 V241 Q242 P243 L246 K249 W252 N255 D256 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 S268 Y271 I274 K275 V276 R277 Q278
L279 L283 T286 T290 E291 V292 I293 E297 E300 L303 N306 R307 P313 G316 V317 Y318 Y319 D320 P321 D324 L325 I326 A327 E328 I329 Q330 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 Y354 A355 D364 V365 K366 Q367 L368 T369 E370
A371 K374 I375 T376 S379 I380 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 Q394 K395 E399 T400 W401 W402 T403 E404 Y405 T409 W410 I411 P412 E415 F416 T419 P420 P421 Y427 GLN LEU GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.70Å 162.80Å 331.80Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29596	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.71	1/4307 (0.0%)	0.98	5/5865 (0.1%)
1	C	0.71	1/4307 (0.0%)	0.98	4/5865 (0.1%)
1	E	0.71	1/4307 (0.0%)	0.98	5/5865 (0.1%)
1	G	0.71	1/4307 (0.0%)	0.98	4/5865 (0.1%)
2	B	0.74	0/3285	1.02	5/4466 (0.1%)
2	D	0.74	0/3285	1.02	5/4466 (0.1%)
2	F	0.74	1/3285 (0.0%)	1.02	5/4466 (0.1%)
2	H	0.74	1/3285 (0.0%)	1.02	5/4466 (0.1%)
All	All	0.72	6/30368 (0.0%)	0.99	38/41324 (0.1%)

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 outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
1	G	0	2
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	12

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	GLN	C-O	5.35	1.33	1.23
1	A	222	GLN	C-O	5.33	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	222	GLN	C-O	5.32	1.33	1.23
1	E	222	GLN	C-O	5.32	1.33	1.23
2	F	24	TRP	CB-CG	-5.02	1.41	1.50

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	94	ILE	C-N-CD	7.79	144.77	128.40
2	F	94	ILE	C-N-CD	7.77	144.72	128.40
2	B	94	ILE	C-N-CD	7.77	144.71	128.40
2	D	94	ILE	C-N-CD	7.76	144.69	128.40
2	D	54	ASN	C-N-CD	-7.01	105.17	120.60

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	TYR	Sidechain
1	A	342	TYR	Sidechain
2	B	61	PHE	Sidechain
1	C	318	TYR	Sidechain
1	C	342	TYR	Sidechain

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	4200	0	4064	338	2
1	C	4200	0	4064	405	24
1	E	4200	0	4064	342	2
1	G	4200	0	4064	401	8
2	B	3198	0	3184	242	4
2	D	3198	0	3184	241	8
2	F	3198	0	3184	245	0
2	H	3198	0	3184	242	20
3	B	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	29596	0	28992	2306	34

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 39.

The worst 5 of 2306 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:PRO:HG3	1:G:326:ILE:CD1	1.22	1.68
1:C:346:PHE:CD1	1:G:390:LYS:CE	1.87	1.58
1:C:345:PRO:CG	1:G:326:ILE:CD1	1.79	1.54
1:C:346:PHE:CD1	1:G:390:LYS:HE3	0.98	1.51
1:C:346:PHE:CE1	1:G:390:LYS:HG3	1.60	1.36

The worst 5 of 34 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:C:54:ASN:CA	2:H:88:TRP:CZ2[3_445]	0.68	1.52
1:C:53:GLU:O	2:H:88:TRP:NE1[3_445]	0.72	1.48
2:D:88:TRP:NE1	1:G:54:ASN:N[3_445]	0.91	1.29
1:C:53:GLU:O	2:H:88:TRP:CD1[3_445]	1.03	1.17
1:C:53:GLU:C	2:H:88:TRP:NE1[3_445]	1.08	1.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	5 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	530/560 (95%)	438 (83%)	75 (14%)	17 (3%)	5 33
1	E	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	5 33
1	G	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	5 33
2	B	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5 34
2	D	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5 34
2	F	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5 34
2	H	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5 34
All	All	3676/4000 (92%)	3035 (83%)	525 (14%)	116 (3%)	5 33

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	345	PRO
2	B	94	ILE
1	C	222	GLN
1	C	345	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	431/500 (86%)	411 (95%)	20 (5%)	33 74
1	C	431/500 (86%)	411 (95%)	20 (5%)	33 74
1	E	431/500 (86%)	410 (95%)	21 (5%)	31 72
1	G	431/500 (86%)	411 (95%)	20 (5%)	33 74
2	B	343/400 (86%)	323 (94%)	20 (6%)	25 66
2	D	343/400 (86%)	323 (94%)	20 (6%)	25 66
2	F	343/400 (86%)	323 (94%)	20 (6%)	25 66
2	H	343/400 (86%)	323 (94%)	20 (6%)	25 66
All	All	3096/3600 (86%)	2935 (95%)	161 (5%)	29 69

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	170	PRO
1	E	252	TRP
2	H	63	ILE
2	D	266	TRP
1	E	4	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	208	HIS
1	E	175	ASN
2	H	145	GLN
2	D	235	HIS
1	E	23	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.