



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 11:48 PM EDT

PDB ID : 2YKQ
Title : Structure of the human LINE-1 ORF1p trimer
Authors : Khazina, E.; Weichenrieder, O.
Deposited on : 2011-05-28
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray 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/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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

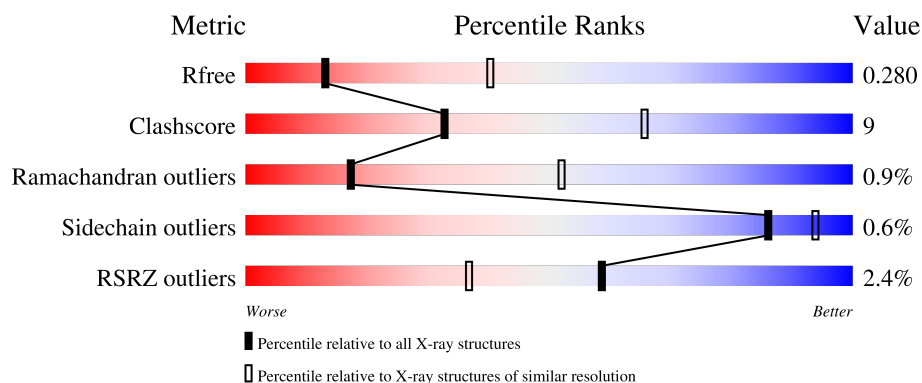
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	229	 2% 64% 22% 13%
1	B	229	 3% 67% 19% 14%
1	C	229	 2% 66% 21% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4948 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 LINE-1 ORF1P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	Se	0	0	0
			1660	1048	302	306	4			
1	B	198	Total	C	N	O	Se	0	0	0
			1632	1034	298	296	4			
1	C	200	Total	C	N	O	Se	0	0	0
			1654	1046	303	301	4			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MSE	CYS	engineered mutation	UNP Q15605
A	105	ALA	ARG	engineered mutation	UNP Q15605
A	327	HIS	-	expression tag	UNP Q15605
A	328	HIS	-	expression tag	UNP Q15605
A	329	HIS	-	expression tag	UNP Q15605
A	330	HIS	-	expression tag	UNP Q15605
A	331	HIS	-	expression tag	UNP Q15605
A	332	HIS	-	expression tag	UNP Q15605
A	121	ALA	MET	engineered mutation	UNP Q15605
A	125	ILE	MET	engineered mutation	UNP Q15605
A	128	ILE	MET	engineered mutation	UNP Q15605
B	104	MSE	CYS	engineered mutation	UNP Q15605
B	105	ALA	ARG	engineered mutation	UNP Q15605
B	327	HIS	-	expression tag	UNP Q15605
B	328	HIS	-	expression tag	UNP Q15605
B	329	HIS	-	expression tag	UNP Q15605
B	330	HIS	-	expression tag	UNP Q15605
B	331	HIS	-	expression tag	UNP Q15605
B	332	HIS	-	expression tag	UNP Q15605
B	121	ALA	MET	engineered mutation	UNP Q15605
B	125	ILE	MET	engineered mutation	UNP Q15605
B	128	ILE	MET	engineered mutation	UNP Q15605
C	104	MSE	CYS	engineered mutation	UNP Q15605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	105	ALA	ARG	engineered mutation	UNP Q15605
C	327	HIS	-	expression tag	UNP Q15605
C	328	HIS	-	expression tag	UNP Q15605
C	329	HIS	-	expression tag	UNP Q15605
C	330	HIS	-	expression tag	UNP Q15605
C	331	HIS	-	expression tag	UNP Q15605
C	332	HIS	-	expression tag	UNP Q15605
C	121	ALA	MET	engineered mutation	UNP Q15605
C	125	ILE	MET	engineered mutation	UNP Q15605
C	128	ILE	MET	engineered mutation	UNP Q15605

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.44Å 91.64Å 107.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.81 – 3.10 69.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.81-3.10) 99.7 (69.80-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.13Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.239 , 0.286 0.239 , 0.280	Depositor DCC
R_{free} test set	671 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4948	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: CL

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	0.22	0/1678	0.37	0/2242
1	B	0.21	0/1650	0.37	0/2205
1	C	0.22	0/1672	0.37	0/2232
All	All	0.22	0/5000	0.37	0/6679

There are no bond length outliers.

There are no bond angle outliers.

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	1660	0	1719	35	0
1	B	1632	0	1692	30	0
1	C	1654	0	1714	33	0
2	A	2	0	0	0	0
All	All	4948	0	5125	88	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 9.

All (88) 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:A:189:LEU:HD23	1:A:226:MSE:HE1	1.62	0.82
1:B:138:ARG:HH22	1:C:140:LYS:HG2	1.45	0.81
1:A:158:LEU:HG	1:A:227:LYS:HG3	1.76	0.67
1:B:127:GLU:O	1:B:131:GLU:HG2	1.96	0.65
1:A:225:GLU:HG3	1:A:229:LYS:HE2	1.78	0.65
1:A:274:LYS:HG3	1:A:316:LEU:HD21	1.79	0.65
1:A:226:MSE:HE3	1:A:230:MSE:HE3	1.80	0.63
1:B:138:ARG:NH2	1:C:140:LYS:HG2	2.15	0.62
1:B:229:LYS:HG2	1:B:232:ARG:HH22	1.65	0.62
1:A:158:LEU:HD21	1:A:231:LEU:HG	1.84	0.60
1:B:160:LEU:HB2	1:B:217:ILE:HB	1.86	0.57
1:C:304:ARG:O	1:C:308:THR:HG23	2.04	0.57
1:C:271:LEU:HD21	1:C:317:LEU:HD11	1.87	0.56
1:B:198:GLN:HB2	1:B:220:ARG:HG2	1.85	0.56
1:C:282:TYR:CD2	1:C:283:PRO:HA	2.40	0.56
1:A:159:ARG:HB2	1:A:250:THR:HG23	1.88	0.56
1:B:146:LEU:HA	1:B:149:ILE:HG22	1.88	0.56
1:A:305:ASP:O	1:A:308:THR:HG22	2.08	0.54
1:C:267:ILE:HG12	1:C:320:ALA:HB1	1.89	0.54
1:A:174:LEU:HB3	1:A:200:ILE:HD13	1.90	0.54
1:B:158:LEU:HD23	1:B:159:ARG:N	2.23	0.54
1:C:124:GLU:O	1:C:128:ILE:HG13	2.08	0.53
1:C:299:ASP:OD1	1:C:302:MSE:HG3	2.08	0.53
1:C:135:ARG:O	1:C:139:ILE:HG13	2.09	0.53
1:A:291:GLU:CD	1:A:310:ARG:HH12	2.12	0.53
1:B:229:LYS:HG2	1:B:232:ARG:NH2	2.24	0.53
1:A:303:LEU:HD23	1:A:321:LEU:HD21	1.91	0.52
1:C:150:TRP:HB3	1:C:254:SER:HB3	1.92	0.52
1:C:185:ASN:ND2	1:C:237:LYS:HE3	2.25	0.52
1:A:149:ILE:HB	1:B:150:TRP:CZ2	2.45	0.51
1:A:159:ARG:HG2	1:A:218:ILE:HD13	1.92	0.51
1:B:178:LEU:O	1:B:182:ILE:HG13	2.10	0.51
1:C:121:ALA:O	1:C:125:ILE:HG13	2.11	0.50
1:B:287:SER:HA	1:B:295:LYS:O	2.11	0.50
1:C:242:LEU:HB2	1:C:247:ILE:HD13	1.94	0.50
1:B:202:ARG:HD3	1:B:217:ILE:HG12	1.94	0.50
1:A:120:ALA:O	1:A:124:GLU:HG2	2.11	0.50
1:A:287:SER:HA	1:A:295:LYS:O	2.12	0.50
1:A:189:LEU:O	1:A:190:ALA:HB3	2.12	0.49
1:B:317:LEU:HB3	1:B:321:LEU:HD13	1.94	0.49
1:A:160:LEU:HB2	1:A:217:ILE:HB	1.94	0.49
1:C:160:LEU:HB2	1:C:217:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLN:HB3	1:C:220:ARG:HG2	1.93	0.48
1:C:274:LYS:HG3	1:C:316:LEU:HD21	1.96	0.48
1:A:147:GLN:HG3	1:A:256:GLU:HB2	1.96	0.48
1:C:185:ASN:HD22	1:C:237:LYS:HE3	1.79	0.48
1:A:197:ILE:O	1:C:223:LYS:HE3	2.14	0.47
1:A:283:PRO:HG2	1:A:284:ALA:H	1.79	0.47
1:A:226:MSE:CE	1:A:230:MSE:HE3	2.44	0.47
1:C:157:ASN:O	1:C:227:LYS:HE3	2.13	0.47
1:A:278:PRO:HA	1:A:287:SER:O	2.14	0.47
1:C:155:ARG:O	1:C:227:LYS:HD2	2.15	0.47
1:A:195:VAL:HG11	1:A:226:MSE:HE2	1.97	0.47
1:C:259:GLN:O	1:C:263:GLU:HG3	2.14	0.47
1:A:149:ILE:O	1:A:153:VAL:HG23	2.15	0.46
1:B:133:LYS:O	1:B:137:LYS:HG2	2.15	0.46
1:C:259:GLN:HA	1:C:262:ARG:HB2	1.97	0.46
1:A:113:GLN:O	1:A:117:ARG:HG3	2.16	0.45
1:C:153:VAL:O	1:C:220:ARG:NH2	2.47	0.45
1:B:155:ARG:HB3	1:B:156:PRO:HD3	1.98	0.45
1:A:114:LEU:HD21	1:B:114:LEU:HB2	1.98	0.45
1:B:145:SER:HB3	1:C:146:LEU:HD13	1.98	0.45
1:B:304:ARG:HG2	1:B:321:LEU:HD23	1.98	0.45
1:B:199:GLU:HG2	1:B:200:ILE:N	2.32	0.44
1:B:185:ASN:HA	1:B:237:LYS:HE3	1.99	0.44
1:A:125:ILE:HG23	1:C:128:ILE:HD11	1.98	0.44
1:A:301:GLN:HA	1:A:304:ARG:HH11	1.83	0.44
1:B:142:ASN:OD1	1:C:143:GLU:HG2	2.18	0.44
1:B:138:ARG:HH22	1:C:140:LYS:CG	2.24	0.44
1:B:200:ILE:HD12	1:B:219:VAL:HG22	2.00	0.43
1:A:256:GLU:H	1:A:256:GLU:CD	2.22	0.43
1:C:150:TRP:CE3	1:C:154:LYS:HE3	2.54	0.43
1:B:121:ALA:O	1:B:125:ILE:HG13	2.18	0.42
1:B:321:LEU:HB3	1:B:323:MSE:HG3	2.01	0.42
1:A:178:LEU:O	1:A:182:ILE:HG13	2.19	0.42
1:C:225:GLU:O	1:C:229:LYS:HG3	2.19	0.42
1:A:174:LEU:HD13	1:A:200:ILE:HG12	2.02	0.42
1:B:282:TYR:CD2	1:B:283:PRO:HA	2.54	0.42
1:B:314:LYS:O	1:B:318:LYS:HB2	2.20	0.42
1:C:307:VAL:O	1:C:314:LYS:HB2	2.20	0.41
1:A:154:LYS:HD3	1:A:252:ASP:CG	2.41	0.41
1:C:281:SER:HB2	1:C:285:LYS:HB2	2.02	0.41
1:B:298:ILE:HD12	1:B:298:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG21	1:C:114:LEU:HD11	2.03	0.41
1:A:140:LYS:HD2	1:A:143:GLU:OE1	2.20	0.40
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.91	0.40
1:A:124:GLU:O	1:A:128:ILE:HG13	2.21	0.40
1:B:124:GLU:O	1:B:128:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

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	194/229 (85%)	186 (96%)	6 (3%)	2 (1%)	15	49
1	B	192/229 (84%)	178 (93%)	12 (6%)	2 (1%)	15	49
1	C	194/229 (85%)	190 (98%)	3 (2%)	1 (0%)	29	64
All	All	580/687 (84%)	554 (96%)	21 (4%)	5 (1%)	17	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	PRO
1	B	168	VAL
1	A	265	GLY
1	C	283	PRO
1	B	283	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	183/204 (90%)	181 (99%)	2 (1%)	73	89
1	B	178/204 (87%)	178 (100%)	0	100	100
1	C	180/204 (88%)	179 (99%)	1 (1%)	86	94
All	All	541/612 (88%)	538 (99%)	3 (1%)	86	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	PHE
1	A	189	LEU
1	C	186	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	C	185	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 ⓘ

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	196/229 (85%)	-0.02	4 (2%) 65 44	37, 68, 111, 154	0
1	B	194/229 (84%)	0.07	6 (3%) 49 26	35, 77, 122, 145	0
1	C	196/229 (85%)	0.13	4 (2%) 65 44	36, 75, 116, 145	0
All	All	586/687 (85%)	0.06	14 (2%) 59 37	35, 73, 116, 154	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	TYR	3.2
1	C	169	GLU	2.9
1	A	239	ARG	2.8
1	C	191	ARG	2.7
1	A	113	GLN	2.7
1	A	194	ASN	2.4
1	B	293	GLU	2.4
1	A	322	ASN	2.2
1	C	168	VAL	2.2
1	C	318	LYS	2.2
1	B	167	ASP	2.1
1	B	213	THR	2.1
1	B	294	ILE	2.1
1	B	168	VAL	2.0

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	CL	A	1325	1/1	0.93	0.26	94,94,94,94	0
2	CL	A	1324	1/1	0.98	0.17	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.