



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2022 – 01:08 pm BST

PDB ID : 7NX0
Title : LTK:ALKAL1 complex stabilized by a Nanobody
Authors : De Munck, S.; Savvides, S.N.
Deposited on : 2021-03-17
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

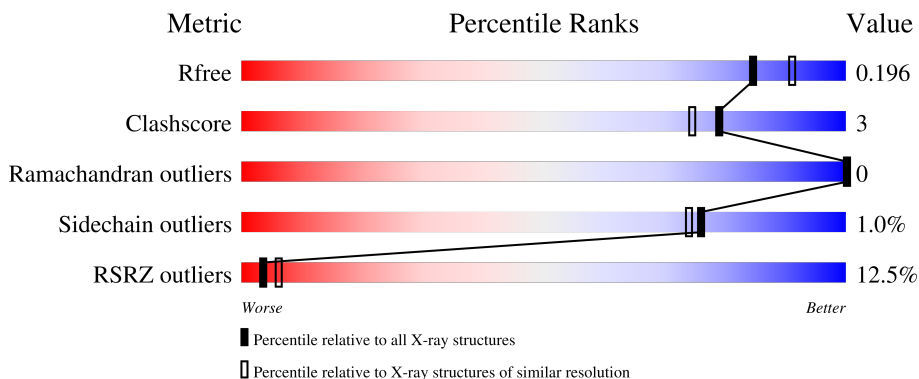
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	B	322	
1	C	322	
2	D	126	
2	E	126	
3	A	79	

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
4	NA	B	401	-	-	-	X
4	NA	B	402	-	-	-	X
4	NA	C	401	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13314 atoms, of which 6128 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 Leukocyte tyrosine kinase receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	C	297	4020	1273	1942	391	408	6	7	1	0
1	B	301	4075	1288	1970	398	412	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	379	GLY	-	expression tag	UNP P29376
C	380	THR	-	expression tag	UNP P29376
C	381	ASP	-	expression tag	UNP P29376
C	382	GLU	-	expression tag	UNP P29376
C	383	VAL	-	expression tag	UNP P29376
C	384	ASP	-	expression tag	UNP P29376
B	379	GLY	-	expression tag	UNP P29376
B	380	THR	-	expression tag	UNP P29376
B	381	ASP	-	expression tag	UNP P29376
B	382	GLU	-	expression tag	UNP P29376
B	383	VAL	-	expression tag	UNP P29376
B	384	ASP	-	expression tag	UNP P29376

- Molecule 2 is a protein called Nb3.16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	D	120	1783	566	868	165	179	5	0	0	0
2	E	123	1800	575	873	167	180	5	0	0	0

- Molecule 3 is a protein called ALK and LTK ligand 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	A	58	954	307	475	87	81	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	-	expression tag	UNP Q6UXT8
A	131	THR	-	expression tag	UNP Q6UXT8
A	132	ASP	-	expression tag	UNP Q6UXT8
A	133	GLU	-	expression tag	UNP Q6UXT8
A	134	VAL	-	expression tag	UNP Q6UXT8
A	135	ASP	-	expression tag	UNP Q6UXT8

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		

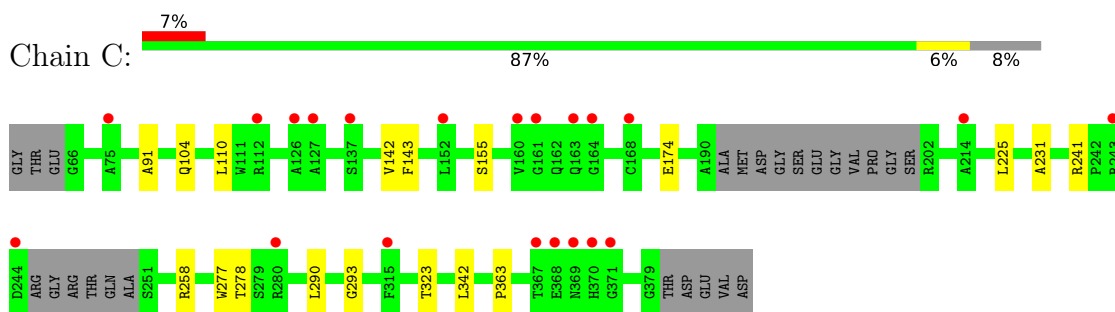
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	270	Total	O	0	0
			270	270		
5	D	116	Total	O	0	0
			116	116		
5	B	207	Total	O	0	0
			207	207		
5	E	55	Total	O	0	0
			55	55		
5	A	30	Total	O	0	0
			30	30		

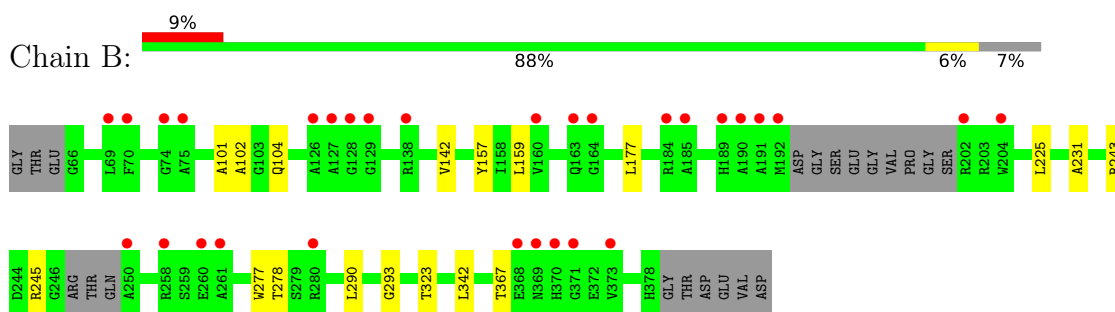
3 Residue-property plots [i](#)

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.

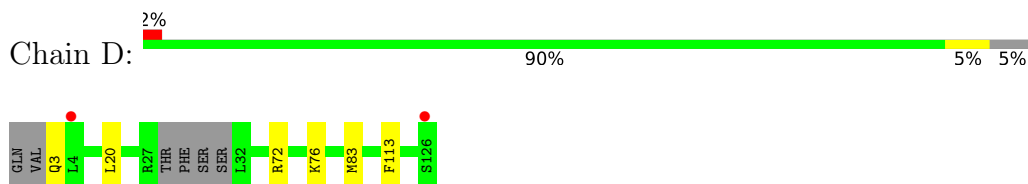
- Molecule 1: Leukocyte tyrosine kinase receptor



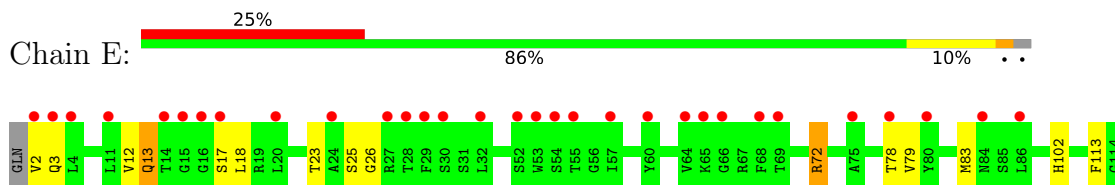
- Molecule 1: Leukocyte tyrosine kinase receptor

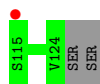


- Molecule 2: Nb3.16

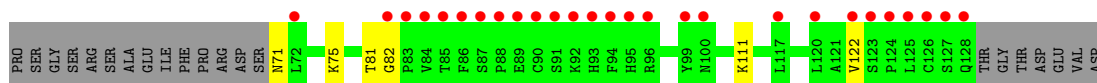


- Molecule 2: Nb3.16





- Molecule 3: ALK and LTK ligand 1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	129.11Å 129.11Å 109.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.26 – 1.95 42.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.26-1.95) 99.7 (42.26-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.95Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.169 , 0.196 0.169 , 0.196	Depositor DCC
R_{free} test set	3778 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.468	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13314	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.34	0/2150	0.59	0/2902
1	C	0.38	0/2126	0.64	0/2871
2	D	0.38	0/934	0.62	0/1261
2	E	0.31	0/947	0.52	0/1282
3	A	0.30	0/493	0.48	0/665
All	All	0.35	0/6650	0.60	0/8981

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 [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	B	2105	1970	1967	11	1
1	C	2078	1942	1940	10	1
2	D	915	868	868	4	0
2	E	927	873	873	9	0
3	A	479	475	475	4	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	207	0	0	1	0
5	C	270	0	0	2	0
5	D	116	0	0	1	1
5	E	55	0	0	0	0
All	All	7186	6128	6123	35	2

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 3.

The worst 5 of 35 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:E:2:VAL:HG23	2:E:3:GLN:HG2	1.72	0.70
3:A:81:THR:HG22	3:A:82:GLY:O	2.01	0.59
1:B:101:ALA:O	1:B:102:ALA:HB2	2.05	0.57
1:B:277:TRP:CD1	1:B:278:THR:HG23	2.42	0.54
1:C:225:LEU:HD12	2:D:113:PHE:CZ	2.42	0.53

All (2) 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)
5:D:263:HOH:O	5:D:298:HOH:O[5_554]	1.98	0.22
1:C:174:GLU:OE2	1:B:245:ARG:HE[3_454]	1.51	0.09

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	B	295/322 (92%)	286 (97%)	9 (3%)	0	100 100
1	C	292/322 (91%)	284 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	116/126 (92%)	114 (98%)	2 (2%)	0	100	100
2	E	121/126 (96%)	119 (98%)	2 (2%)	0	100	100
3	A	56/79 (71%)	56 (100%)	0	0	100	100
All	All	880/975 (90%)	859 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	191/208 (92%)	190 (100%)	1 (0%)	88	88
1	C	189/208 (91%)	188 (100%)	1 (0%)	88	88
2	D	96/102 (94%)	95 (99%)	1 (1%)	76	74
2	E	95/102 (93%)	92 (97%)	3 (3%)	39	27
3	A	54/72 (75%)	54 (100%)	0	100	100
All	All	625/692 (90%)	619 (99%)	6 (1%)	76	74

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	13	GLN
2	E	25	SER
2	E	72	ARG
2	D	72	ARG
1	C	241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	301/322 (93%)	0.69	30 (9%) 7 11	36, 48, 71, 111	0
1	C	297/322 (92%)	0.65	21 (7%) 16 24	28, 37, 61, 98	0
2	D	120/126 (95%)	0.10	2 (1%) 70 77	31, 44, 78, 117	0
2	E	123/126 (97%)	1.44	32 (26%) 0 0	51, 78, 110, 128	0
3	A	58/79 (73%)	2.19	27 (46%) 0 0	47, 65, 96, 111	0
All	All	899/975 (92%)	0.80	112 (12%) 3 6	28, 46, 90, 128	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	10.3
3	A	90	CYS	8.5
3	A	128	GLN	6.3
2	E	29	PHE	6.2
3	A	125	LEU	5.5

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 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(Å ²)	Q<0.9
4	NA	B	401	1/1	0.59	2.94	137,137,137,137	0
4	NA	B	402	1/1	0.71	0.64	105,105,105,105	0
4	NA	C	401	1/1	0.74	1.44	119,119,119,119	0
4	NA	C	402	1/1	0.85	1.01	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.