



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2021 – 01:05 pm BST

PDB ID : 7NX3
Title : Crystal structure of ALK in complex with Fab324
Authors : De Munck, S.; Savvides, S.N.
Deposited on : 2021-03-17
Resolution : 2.81 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

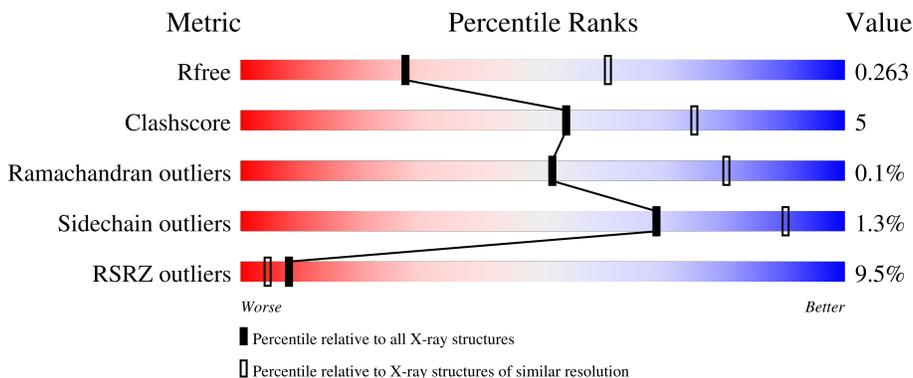
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	389	
1	F	389	
2	B	231	
2	E	231	
3	C	218	

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Mol	Chain	Length	Quality of chain
3	D	218	<p>12% 87% 12%</p>

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	NAG	A	1103	-	-	-	X
4	NAG	A	1104	-	-	-	X
4	NAG	F	1103	-	-	-	X
4	NAG	F	1104	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21043 atoms, of which 10284 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 ALK tyrosine kinase receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	292	4037	1286	1961	367	410	13	0	0	0
1	F	293	4045	1289	1964	368	411	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1031	GLY	-	expression tag	UNP Q9UM73
A	1032	THR	-	expression tag	UNP Q9UM73
A	1033	ASP	-	expression tag	UNP Q9UM73
A	1034	GLU	-	expression tag	UNP Q9UM73
A	1035	VAL	-	expression tag	UNP Q9UM73
A	1036	ASP	-	expression tag	UNP Q9UM73
F	1031	GLY	-	expression tag	UNP Q9UM73
F	1032	THR	-	expression tag	UNP Q9UM73
F	1033	ASP	-	expression tag	UNP Q9UM73
F	1034	GLU	-	expression tag	UNP Q9UM73
F	1035	VAL	-	expression tag	UNP Q9UM73
F	1036	ASP	-	expression tag	UNP Q9UM73

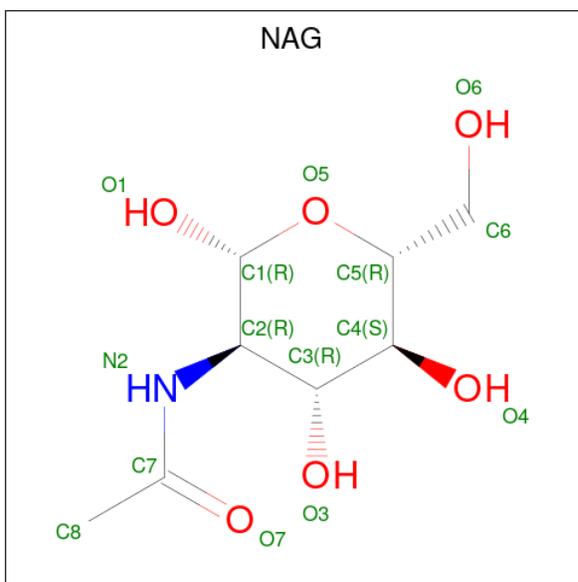
- Molecule 2 is a protein called Fab324 HeavyChain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	209	3105	1002	1530	255	312	6	0	0	0
2	E	212	3148	1016	1553	258	315	6	0	0	0

- Molecule 3 is a protein called Fab324 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	216	Total 3242	C 1035	H 1582	N 282	O 335	S 8	0	0	0
3	D	216	Total 3242	C 1035	H 1582	N 282	O 335	S 8	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	F	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	F	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	F	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	F	1	Total 28	C 8	H 14	N 1	O 5	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	109.70Å 137.47Å 144.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.81 49.76 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.04-2.81) 99.1 (49.76-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.228 , 0.266 0.226 , 0.263	Depositor DCC
R_{free} test set	2010 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtrriage
Anisotropy	0.454	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21043	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8135e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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:
NAG

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	0.31	0/2123	0.57	0/2869
1	F	0.34	0/2128	0.57	0/2876
2	B	0.29	0/1618	0.55	0/2208
2	E	0.31	0/1639	0.54	0/2238
3	C	0.31	0/1699	0.54	0/2306
3	D	0.30	0/1699	0.54	0/2306
All	All	0.31	0/10906	0.55	0/14803

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	A	2076	1961	1957	20	0
1	F	2081	1964	1957	20	2
2	B	1575	1530	1530	16	0
2	E	1595	1553	1553	15	2
3	C	1660	1582	1579	25	0
3	D	1660	1582	1579	19	0
4	A	56	56	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	56	56	52	0	0
All	All	10759	10284	10259	111	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 5.

The worst 5 of 111 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:C:124:PRO:HB2	3:C:129:LEU:HD11	1.62	0.80
2:E:146:LEU:HD13	2:E:218:ILE:CD1	2.12	0.80
3:C:125:SER:O	3:C:129:LEU:HD13	1.83	0.78
1:F:777:GLN:N	1:F:921:PHE:O	2.20	0.75
3:C:124:PRO:HD3	3:C:136:VAL:HG22	1.68	0.75

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)
2:E:211:SER:O	1:F:727:LYS:NZ[4_555]	1.96	0.24
2:E:211:SER:O	1:F:727:LYS:HZ1[4_555]	1.52	0.08

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	288/389 (74%)	281 (98%)	7 (2%)	0	100	100
1	F	289/389 (74%)	281 (97%)	8 (3%)	0	100	100
2	B	205/231 (89%)	200 (98%)	4 (2%)	1 (0%)	29	59
2	E	208/231 (90%)	200 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	214/218 (98%)	207 (97%)	7 (3%)	0	100	100
3	D	214/218 (98%)	208 (97%)	6 (3%)	0	100	100
All	All	1418/1676 (85%)	1377 (97%)	40 (3%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123	LYS

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	206/297 (69%)	201 (98%)	5 (2%)	49	80
1	F	206/297 (69%)	202 (98%)	4 (2%)	57	84
2	B	178/193 (92%)	176 (99%)	2 (1%)	73	91
2	E	180/193 (93%)	177 (98%)	3 (2%)	60	86
3	C	186/190 (98%)	186 (100%)	0	100	100
3	D	186/190 (98%)	185 (100%)	1 (0%)	88	96
All	All	1142/1360 (84%)	1127 (99%)	15 (1%)	69	90

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	27	GLU
1	F	901	THR
2	E	39	GLN
1	F	967	THR
1	F	709	ASN

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](#)

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
4	NAG	A	1101	1	14,14,15	0.33	0	17,19,21	0.66	1 (5%)
4	NAG	A	1104	1	14,14,15	1.53	2 (14%)	17,19,21	0.92	2 (11%)
4	NAG	F	1101	1	14,14,15	1.27	1 (7%)	17,19,21	0.82	0
4	NAG	A	1103	-	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	F	1102	1	14,14,15	0.56	0	17,19,21	1.37	3 (17%)
4	NAG	A	1102	1	14,14,15	0.25	0	17,19,21	0.69	0
4	NAG	F	1104	1	14,14,15	1.57	2 (14%)	17,19,21	0.94	2 (11%)
4	NAG	F	1103	1	14,14,15	0.46	0	17,19,21	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1101	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1104	1	-	3/6/23/26	0/1/1/1
4	NAG	F	1101	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1103	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1102	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1102	1	-	3/6/23/26	0/1/1/1
4	NAG	F	1104	1	-	3/6/23/26	0/1/1/1
4	NAG	F	1103	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1104	NAG	O5-C1	5.26	1.52	1.43
4	A	1104	NAG	O5-C1	5.26	1.52	1.43
4	F	1101	NAG	O5-C1	-4.35	1.36	1.43
4	F	1104	NAG	C1-C2	2.41	1.55	1.52
4	A	1104	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1102	NAG	C1-O5-C5	-4.06	106.69	112.19
4	F	1102	NAG	C2-N2-C7	2.38	126.29	122.90
4	A	1101	NAG	C1-O5-C5	2.35	115.38	112.19
4	F	1104	NAG	C1-C2-N2	2.32	114.46	110.49
4	A	1104	NAG	C1-C2-N2	2.24	114.32	110.49

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1101	NAG	C8-C7-N2-C2
4	F	1101	NAG	O7-C7-N2-C2
4	A	1102	NAG	C1-C2-N2-C7
4	F	1102	NAG	C1-C2-N2-C7
4	A	1104	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	A	292/389 (75%)	0.36	5 (1%) 70 63	17, 32, 61, 89	0
1	F	293/389 (75%)	0.34	2 (0%) 87 84	14, 31, 65, 106	0
2	B	209/231 (90%)	0.94	35 (16%) 1 1	19, 46, 121, 149	0
2	E	212/231 (91%)	0.72	24 (11%) 5 3	20, 43, 107, 139	0
3	C	216/218 (99%)	0.96	44 (20%) 1 0	17, 47, 120, 147	0
3	D	216/218 (99%)	0.77	26 (12%) 4 2	15, 39, 122, 158	0
All	All	1438/1676 (85%)	0.65	136 (9%) 8 4	14, 36, 111, 158	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	160	GLN	9.2
2	B	168	SER	7.3
3	C	134	ALA	6.3
2	E	194	SER	6.1
3	C	160	GLN	5.8

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	NAG	F	1101	14/15	0.46	0.40	64,74,87,89	0
4	NAG	A	1104	14/15	0.48	0.74	40,53,63,64	0
4	NAG	F	1103	14/15	0.49	0.53	41,53,65,65	0
4	NAG	A	1103	14/15	0.55	0.59	55,60,71,72	0
4	NAG	F	1104	14/15	0.68	0.59	41,50,60,62	0
4	NAG	A	1101	14/15	0.73	0.40	55,62,75,75	0
4	NAG	A	1102	14/15	0.89	0.28	32,44,54,54	0
4	NAG	F	1102	14/15	0.89	0.36	36,45,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.