



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2025 – 04:19 pm GMT

PDB ID : 9G9N  
Title : Lipid III flippase Wzx E with NB10 and NB7 nanobodies in inward-facing conformation - crystal 1  
Authors : Le Bas, A.; Naismith, J.H.  
Deposited on : 2024-07-25  
Resolution : 2.80 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](mailto: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
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

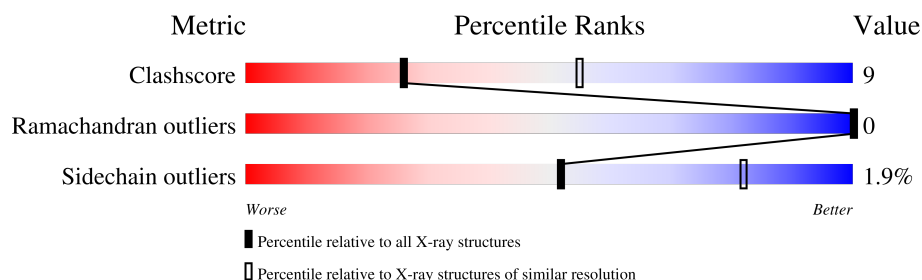
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	425	75% 22% .
2	B	140	74% 16% . 9%
3	C	136	65% 24% . 10%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5060 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 Lipid III flippase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3140	2087	514	526	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AAA7
A	1	VAL	-	cloning artifact	UNP P0AAA7
A	417	LEU	-	expression tag	UNP P0AAA7
A	418	GLU	-	expression tag	UNP P0AAA7
A	419	GLU	-	expression tag	UNP P0AAA7
A	420	ASN	-	expression tag	UNP P0AAA7
A	421	LEU	-	expression tag	UNP P0AAA7
A	422	TYR	-	expression tag	UNP P0AAA7
A	423	PHE	-	expression tag	UNP P0AAA7
A	424	GLN	-	expression tag	UNP P0AAA7

- Molecule 2 is a protein called NB10 Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			960	597	174	185	4			

- Molecule 3 is a protein called NB7 Nanobody.

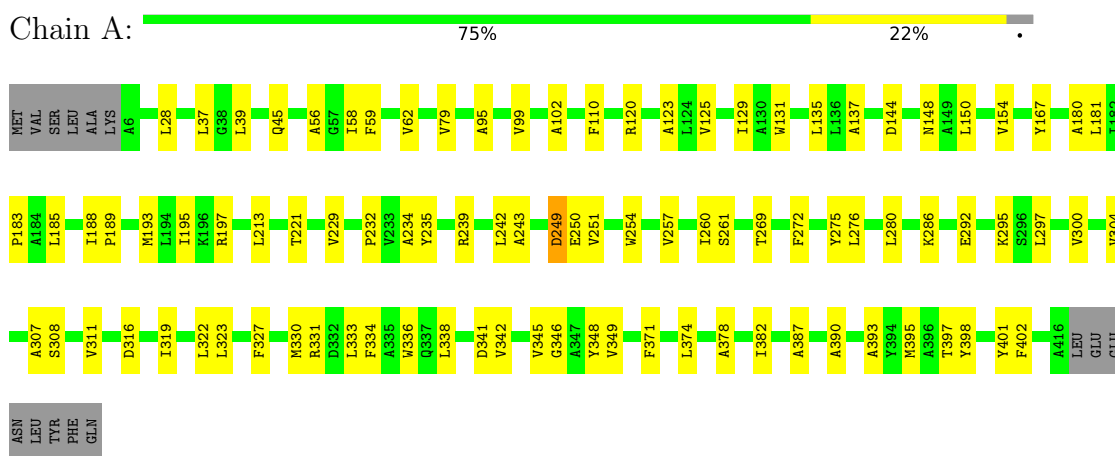
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	123	Total	C	N	O	S	0	0	0
			960	607	165	183	5			

### 3 Residue-property plots

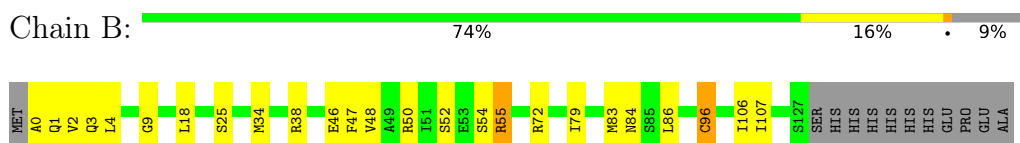
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 failed to run properly.

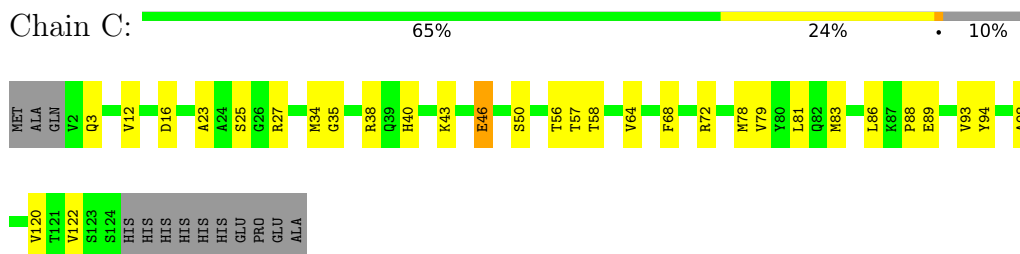
- Molecule 1: Lipid III flippase



- Molecule 2: NB10 Nanobody



- Molecule 3: NB7 Nanobody



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.24Å 191.91Å 101.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.40 – 2.80	Depositor
% Data completeness (in resolution range)	99.7 (32.40-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.256 , 0.313	Depositor
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.852	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5060	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 4.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.25	0/3212	0.46	0/4374
2	B	0.26	0/980	0.52	0/1329
3	C	0.27	0/985	0.50	0/1334
All	All	0.25	0/5177	0.48	0/7037

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	3140	0	3301	58	0
2	B	960	0	930	15	0
3	C	960	0	909	26	0
All	All	5060	0	5140	95	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 (95) 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:269:THR:HA	1:A:272:PHE:HD2	1.54	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HG	1:A:280:LEU:HD11	1.73	0.69
1:A:304:VAL:HG13	1:A:342:VAL:HG22	1.77	0.65
1:A:272:PHE:HE1	1:A:349:VAL:HG12	1.60	0.65
3:C:64:VAL:HG13	3:C:68:PHE:HD2	1.61	0.65
1:A:249:ASP:HB2	3:C:56:THR:HB	1.81	0.62
1:A:125:VAL:HG11	1:A:180:ALA:HB1	1.83	0.61
1:A:99:VAL:HA	1:A:120:ARG:HG2	1.82	0.60
1:A:242:LEU:HD23	1:A:251:VAL:HG22	1.84	0.59
1:A:250:GLU:HG3	1:A:387:ALA:HB2	1.85	0.58
1:A:234:ALA:HB2	1:A:371:PHE:HD2	1.69	0.58
1:A:393:ALA:O	1:A:397:THR:HG23	2.04	0.57
1:A:316:ASP:OD1	1:A:331:ARG:NH1	2.38	0.56
1:A:56:ALA:O	1:A:221:THR:OG1	2.20	0.56
1:A:346:GLY:HA3	1:A:402:PHE:HE1	1.70	0.56
2:B:34:MET:HB3	2:B:79:ILE:HD13	1.88	0.55
1:A:260:ILE:HG12	1:A:322:LEU:HD12	1.89	0.55
3:C:68:PHE:HB3	3:C:81:LEU:HD11	1.89	0.55
3:C:40:HIS:HB2	3:C:43:LYS:HB2	1.90	0.54
1:A:327:PHE:O	1:A:330:MET:HG3	2.07	0.54
2:B:83:MET:HB3	2:B:86:LEU:HD11	1.89	0.53
3:C:64:VAL:HG13	3:C:68:PHE:CD2	2.43	0.52
3:C:23:ALA:HA	3:C:78:MET:HG2	1.92	0.52
1:A:45:GLN:NE2	1:A:232:PRO:HA	2.25	0.52
1:A:292:GLU:HA	1:A:295:LYS:HG2	1.93	0.51
1:A:45:GLN:NE2	1:A:235:TYR:HB2	2.25	0.51
3:C:88:PRO:HA	3:C:122:VAL:HG13	1.91	0.51
3:C:68:PHE:HD1	3:C:83:MET:HA	1.76	0.50
1:A:243:ALA:HB2	1:A:251:VAL:HG21	1.94	0.50
3:C:34:MET:HG3	3:C:79:VAL:HG21	1.94	0.50
1:A:319:ILE:HG12	1:A:330:MET:HE3	1.93	0.50
2:B:38:ARG:HG3	2:B:46:GLU:HG3	1.94	0.49
1:A:374:LEU:HD23	1:A:397:THR:HG21	1.94	0.49
1:A:345:VAL:O	1:A:348:TYR:HB2	2.12	0.49
3:C:94:TYR:HE2	3:C:120:VAL:HB	1.78	0.49
1:A:323:LEU:HD12	1:A:330:MET:HE1	1.95	0.48
3:C:94:TYR:CE2	3:C:120:VAL:HB	2.48	0.48
3:C:99:LYS:HG3	3:C:110:ASP:O	2.14	0.48
1:A:322:LEU:O	1:A:323:LEU:HD23	2.14	0.48
1:A:129:ILE:HD11	1:A:183:PRO:HG2	1.96	0.47
1:A:308:SER:HB3	1:A:338:LEU:HB3	1.96	0.47
1:A:150:LEU:O	1:A:154:VAL:HG23	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD23	1:A:37:LEU:HD12	1.96	0.47
1:A:254:TRP:O	1:A:257:VAL:HG22	2.15	0.47
1:A:272:PHE:CZ	1:A:300:VAL:HG11	2.49	0.47
1:A:330:MET:HA	1:A:333:LEU:HD13	1.95	0.47
2:B:0:ALA:HB3	3:C:57:THR:HG23	1.96	0.47
1:A:181:LEU:HB3	1:A:185:LEU:HD13	1.97	0.47
3:C:98:ALA:HB3	3:C:113:TYR:HB2	1.97	0.47
1:A:144:ASP:OD1	1:A:197:ARG:NH2	2.48	0.46
1:A:382:ILE:HD11	1:A:390:ALA:HB2	1.98	0.46
2:B:52:SER:O	2:B:72:ARG:NH1	2.48	0.46
1:A:336:TRP:HA	1:A:395:MET:HE3	1.97	0.46
3:C:83:MET:HB2	3:C:86:LEU:HD11	1.98	0.45
1:A:45:GLN:HE21	1:A:232:PRO:HA	1.82	0.45
1:A:95:ALA:HA	1:A:123:ALA:HB1	1.99	0.45
3:C:12:VAL:O	3:C:122:VAL:HA	2.15	0.45
1:A:234:ALA:HB2	1:A:371:PHE:CD2	2.50	0.45
3:C:68:PHE:CD1	3:C:83:MET:HA	2.51	0.45
1:A:398:TYR:HA	1:A:401:TYR:HB3	1.99	0.44
1:A:59:PHE:HB3	1:A:137:ALA:HB2	1.99	0.44
1:A:79:VAL:HG12	1:A:213:LEU:HD22	1.99	0.44
2:B:54:SER:OG	2:B:55:ARG:HD2	2.17	0.44
1:A:39:LEU:HD22	1:A:110:PHE:HD1	1.82	0.44
2:B:47:PHE:HE1	2:B:50:ARG:HB3	1.83	0.44
1:A:102:ALA:HB2	1:A:120:ARG:HG3	1.99	0.44
3:C:3:GLN:H	3:C:25:SER:HB3	1.83	0.43
1:A:378:ALA:HB1	1:A:382:ILE:HG13	2.01	0.43
1:A:307:ALA:O	1:A:311:VAL:HG13	2.19	0.43
1:A:334:PHE:O	1:A:338:LEU:HG	2.18	0.43
2:B:38:ARG:HG2	2:B:48:VAL:CG2	2.49	0.43
3:C:38:ARG:NE	3:C:46:GLU:OE2	2.32	0.43
2:B:1:GLN:HG3	2:B:2:VAL:HG23	2.01	0.43
2:B:3:GLN:NE2	3:C:58:THR:O	2.46	0.43
2:B:84:ASN:HD22	2:B:84:ASN:HA	1.63	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.83	0.42
3:C:27:ARG:HD2	3:C:27:ARG:HA	1.84	0.42
3:C:68:PHE:CE1	3:C:83:MET:HB3	2.54	0.42
1:A:188:ILE:HB	1:A:189:PRO:HD3	2.01	0.42
1:A:131:TRP:O	1:A:135:LEU:HD13	2.19	0.42
1:A:229:VAL:O	1:A:229:VAL:HG12	2.19	0.42
2:B:9:GLY:HA2	2:B:18:LEU:HD21	2.02	0.41
2:B:25:SER:HB2	3:C:68:PHE:O	2.19	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD13	2:B:96:CYS:SG	2.60	0.41
2:B:106:ILE:HG22	2:B:107:ILE:HG23	2.02	0.41
1:A:235:TYR:O	1:A:239:ARG:HG3	2.19	0.41
1:A:235:TYR:HB3	1:A:239:ARG:NH1	2.35	0.41
1:A:58:ILE:O	1:A:62:VAL:HG23	2.20	0.41
3:C:89:GLU:OE2	3:C:89:GLU:N	2.40	0.41
1:A:257:VAL:CG1	1:A:330:MET:HB3	2.50	0.41
1:A:195:ILE:HD13	1:A:195:ILE:HA	1.95	0.41
3:C:35:GLY:HA2	3:C:50:SER:HA	2.02	0.41
1:A:193:MET:O	1:A:197:ARG:HB2	2.19	0.40
1:A:261:SER:HB2	1:A:341:ASP:OD2	2.21	0.40
3:C:38:ARG:HA	3:C:93:VAL:O	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	409/425 (96%)	397 (97%)	12 (3%)	0	100	100
2	B	126/140 (90%)	122 (97%)	4 (3%)	0	100	100
3	C	121/136 (89%)	114 (94%)	7 (6%)	0	100	100
All	All	656/701 (94%)	633 (96%)	23 (4%)	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	A	321/334 (96%)	316 (98%)	5 (2%)	58	85
2	B	98/109 (90%)	96 (98%)	2 (2%)	50	81
3	C	98/109 (90%)	95 (97%)	3 (3%)	35	69
All	All	517/552 (94%)	507 (98%)	10 (2%)	52	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	167	TYR
1	A	249	ASP
1	A	275	TYR
1	A	286	LYS
2	B	55	ARG
2	B	96	CYS
3	C	16	ASP
3	C	46	GLU
3	C	72	ARG

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	45	GLN
2	B	84	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.