

# Full wwPDB X-ray Structure Validation Report (i)

#### Jul 19, 2021 – 06:01 pm BST

PDB ID : 7NJZ

Title: X-ray crystallography study of RoAb13 which binds to PIYDIN, a part of the

CCR5 N terminal domain

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Deposited on : 2021-02-17

Resolution : 3.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.22

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)

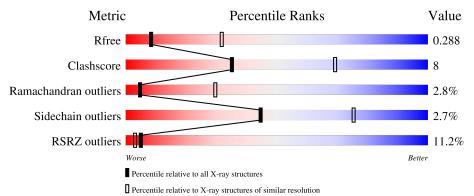
Validation Pipeline (wwPDB-VP) : 2.22

# 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	$1253 \ (3.20 - 3.20)$
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	Н	224	6%	82%	13% • •		
2	L	220	16%	73%	22% • •		
3	С	6	33%	50%	17%		



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3346 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 Antibody RoAb13 Heavy Chain.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Н	218	Total 1645	C 1032	N 281	O 325	S 7	0	0	0

• Molecule 2 is a protein called Antibody RoAb13 Light Chain.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	${f AltConf}$	Trace		
2	L	214	Total 1628	C 1018	N 268	O 333	S	0	0	0

• Molecule 3 is a protein called Region from C-C chemokine receptor type 5 N-terminal domain.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	С	6	Total C N O 51 34 7 10	0	0	0

• Molecule 4 is water.

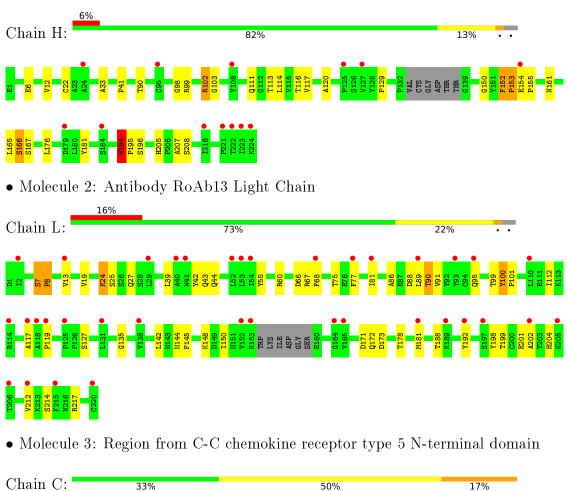
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	11	Total O 11 11	0	0
4	L	11	Total O 11 11	0	0



# 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: Antibody RoAb13 Heavy Chain





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	76.44Å 76.44Å 268.64Å	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.52 - 3.20	Depositor
Resolution (A)	73.52 - 3.20	EDS
% Data completeness	99.9 (73.52-3.20)	Depositor
(in resolution range)	99.9 (73.52-3.20)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.59  (at  3.19Å)	Xtriage
Refinement program	REFMAC 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
$R, R_{free}$	0.269 , $0.292$	Depositor
it, it free	0.273 , $0.288$	DCC
$R_{free}$ test set	707  reflections  (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	122.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35 , 133.8	EDS
L-test for twinning <sup>2</sup>	$< L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

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	
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	Н	0.25	0/1683	0.48	0/2289
2	L	0.26	0/1664	0.47	0/2264
3	С	0.33	0/52	0.65	0/70
All	All	0.26	0/3399	0.48	0/4623

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	Н	0	2
2	L	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	${f Res}$	$\mathbf{Type}$	Group
1	Н	152	PHE	Peptide
1	Н	194	TRP	Peptide
2	L	100	TYR	Peptide

### 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	Н	1645	0	1604	19	0
2	L	1628	0	1530	34	0
3	С	51	0	48	4	0
4	Н	11	0	0	0	0
4	L	11	0	0	0	0
All	All	3346	0	3182	53	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 8.

All (53) 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:H:194:TRP:O	1:H:196:SER:N	2.19	0.76
3:C:9:ILE:HD12			
2:L:90:THR:OG1	3:C:12:ILE:HD11	$\frac{1.70}{2.22}$	0.72
	2:L:91:VAL:N		0.71
2:L:135:GLY:HA2	2:L:188:THR:HA	1.81	0.63
2:L:117:ALA:HB3	2:L:145:PHE:HA	1.82	0.61
2:L:150:ILE:HD11	2:L:202:ALA:HB1	1.80	0.61
2:L:19:VAL:HB	2:L:81:ILE:HB	1.83	0.60
2:L:145:PHE:N	2:L:178:THR:OG1	2.36	0.58
2:L:60:ARG:NH1	2:L:68:PHE:O	2.35	0.58
1:H:153:PRO:HD2	1:H:205:HIS:NE2	2.19	0.57
2:L:43:GLN:HG3	2:L:90:THR:HG21	1.86	0.56
2:L:119:PRO:HB2	2:L:142:LEU:HD12	1.87	0.56
1:H:205:HIS:CE1	1:H:208:SER:HG	2.23	0.56
2:L:150:ILE:HB	2:L:204:HIS:CD2	2.41	0.56
2:L:99:THR:HG21	3:C:11:ASP:H	1.70	0.56
2:L:142:LEU:HB2	2:L:181:MET:HB2	1.87	0.55
1:H:114:LEU:HD12	1:H:155:PRO:HD3	1.88	0.55
2:L:199:THR:HG23	2:L:214:SER:HB2	1.88	0.55
2:L:67:ARG:NH1	2:L:88:ASP:OD2	2.41	0.53
2:L:13:VAL:HG21	2:L:19:VAL:HG22	1.91	0.51
2:L:198:TYR:O	2:L:214:SER:OG	2.18	0.51
1:H:166:SER:OG	1:H:167:SER:N	2.44	0.51
1:H:99:ARG:NH2	2:L:55:TYR:OH	2.34	0.51
1:H:6:GLU:HB3	1:H:113:THR:HB	1.93	0.51
2:L:42:TYR:HE2	2:L:95:GLN:HE21	1.58	0.51
2:L:192:TYR:O	2:L:198:TYR:OH	2.28	0.50
2:L:44:GLN:O	2:L:90:THR:OG1	2.25	0.50
1:H:114:LEU:HD11	1:H:116:THR:HG23	1.96	0.48
1:H:12:VAL:HG23	1:H:117:VAL:HG12	1.95	0.48



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A		Interatomic	Clash
Atom-1	Atom-2	${f distance}({f \AA})$	overlap (Å)
1:H:120:ALA:HB3	1:H:152:PHE:CE2	2.48	0.48
2:L:99:THR:CG2	3:C:11:ASP:H	2.27	0.47
1:H:102:ARG:HD2	1:H:103:GLY:N	2.30	0.47
1:H:161:ASN:HB2	1:H:165:LEU:HD23	1.97	0.46
2:L:25:SER:HB3	2:L:75:THR:HA	1.96	0.46
2:L:7:SER:OG	2:L:8:PRO:HD2	2.16	0.46
1:H:129:PRO:O	2:L:127:SER:HB3	2.16	0.46
2:L:86:ALA:O	2:L:89:LEU:HG	2.15	0.46
2:L:89:LEU:HD21	2:L:112:ILE:HD12	1.98	0.46
1:H:33:ALA:O	1:H:98:GLY:N	2.43	0.45
2:L:112:ILE:HG22	2:L:172:GLN:OE1	2.17	0.45
1:H:205:HIS:ND1	1:H:208:SER:OG	2.48	0.45
1:H:41:PRO:HD3	1:H:90:THR:O	2.17	0.45
2:L:201:GLU:HG3	2:L:212:VAL:HG12	1.99	0.44
2:L:24:LYS:HE3	2:L:24:LYS:HB3	1.71	0.44
1:H:154:GLU:HG2	1:H:181:TYR:CZ	2.53	0.43
3:C:9:ILE:HD12	3:C:12:ILE:CD1	2.43	0.43
2:L:150:ILE:HD12	2:L:204:HIS:CG	2.53	0.43
1:H:6:GLU:HB2	1:H:111:GLN:HE22	1.83	0.42
2:L:145:PHE:HB2	2:L:204:HIS:HE1	1.84	0.42
2:L:27:GLN:HE21	2:L:27:GLN:HB2	1.69	0.42
2:L:39:LEU:HD13	2:L:77:PHE:CD1	2.56	0.41
2:L:67:ARG:H	2:L:67:ARG:HG2	1.75	0.41
1:H:176:LEU:HB2	1:H:181:TYR:CE1	2.56	0.41

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	Н	214/224 (96%)	192 (90%)	16 (8%)	6 (3%)	5 29



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	210/220 (96%)	186 (89%)	19 (9%)	5 (2%)	6 34
3	С	4/6 (67%)	1 (25%)	2 (50%)	1 (25%)	0 0
All	All	428/450 (95%)	379 (89%)	37 (9%)	12 (3%)	5 29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Н	194	TRP
1	Н	195	PRO
1	Н	207	ALA
2	L	8	PRO
2	L	101	PRO
1	Н	153	PRO
1	Н	166	SER
2	L	100	TYR
2	L	90	THR
3	С	11	ASP
1	Н	150	GLY
2	L	144	ASN

#### 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	Н	185/191 (97%)	183 (99%)	2 (1%)	73 88
2	L	182/196 (93%)	175 (96%)	7 (4%)	33 67
3	С	6/6 (100%)	5 (83%)	1 (17%)	2 10
All	All	373/393 (95%)	363 (97%)	10 (3%)	44 75

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

$\mathbf{M}$	ol	Chain	Res	Type
1		Н	22	CYS
1		Н	102	ARG



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Mol	Chain	Res	Type
2	L	7	SER
2	L	24	LYS
2	L	66	ASP
2	L	148	LYS
2	L	171	ASP
2	L	173	ASP
2	L	217	ARG
3	С	10	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	27	GLN
2	L	48	GLN
2	L	95	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	Н	218/224 (97%)	0.80	13 (5%) 21 12	64, 108, 147, 214	0
2	L	214/220 (97%)	0.98	36 (16%) 1 1	84, 132, 180, 231	0
3	С	6/6 (100%)	0.80	0 100 100	121, 134, 135, 143	6 (100%)
All	All	438/450 (97%)	0.89	49 (11%) 5 3	64, 117, 172, 231	6 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	223	ILE	11.8
1	Н	222	THR	11.3
2	L	220	CYS	11.1
2	L	206	THR	6.9
2	L	205	LYS	5.6
1	Н	224	LYS	4.4
2	L	202	ALA	4.1
2	L	152	VAL	3.8
2	L	189	LYS	3.6
2	L	119	PRO	3.4
2	L	95	GLN	3.3
2	L	2	ILE	3.0
2	L	41	TRP	2.9
2	L	215	PHE	2.9
2	L	192	TYR	2.9
2	L	29	LEU	2.8
2	L	197	SER	2.7
1	Н	179	ASP	2.5
2	L	54	ILE	2.5
1	Н	125	PRO	2.5
2	L	117	ALA	2.4
1	Н	95	CYS	2.4
2	L	13	VAL	2.4



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Mol	Chain	Res	Type	RSRZ
2	L	165	VAL	2.4
1	Н	216	ILE	2.4
2	L	118	ALA	2.4
2	L	40	ALA	2.4
1	Н	108	TYR	2.4
2	L	68	PHE	2.4
2	L	153	LYS	2.3
2	L	114	ARG	2.3
2	L	212	VAL	2.3
1	Н	24	ALA	2.3
2	L	93	TYR	2.3
2	L	164	GLY	2.3
1	Н	154	GLU	2.2
1	Н	221	PRO	2.2
2	L	89	LEU	2.2
2	L	53	LEU	2.1
2	L	77	PHE	2.1
2	L	125	PRO	2.1
2	L	181	MET	2.1
2	L	138	VAL	2.1
2	L	81	ILE	2.1
2	L	52	LEU	2.0
2	L	131	LEU	2.0
1	Н	184	SER	2.0
2	L	110	LEU	2.0
1	Н	127	VAL	2.0

### 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)

There are no ligands in this entry.



# 6.5 Other polymers (i)

There are no such residues in this entry.

