



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 03:53 AM BST

PDB ID : 6WN4  
Title : Structural basis for the binding of monoclonal antibody 5D2 to the tryptophan-rich lipid-binding loop in lipoprotein lipase  
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Deposited on : 2020-04-22  
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.

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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	:	2.13.1
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)	:	2.13.1

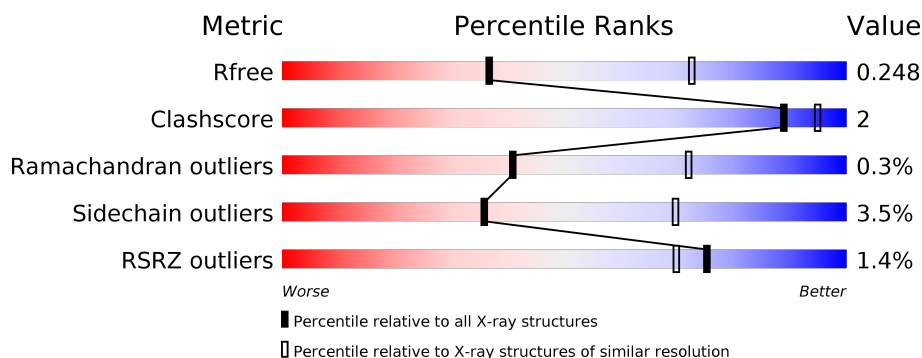
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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  $\leq 5\%$ . 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	222	<div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	H	222	<div> <div>3%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
2	B	214	<div> <div>%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
2	L	214	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
3	C	14	<div> <div>79%</div> <div>21%</div> </div>
3	D	14	<div> <div>79%</div> <div>21%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6822 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 5D2 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1659	1063	267	323	6			
1	H	221	Total	C	N	O	S	0	0	0
			1703	1086	277	334	6			

- Molecule 2 is a protein called 5D2 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1594	993	265	327	9			
2	L	212	Total	C	N	O	S	0	0	0
			1627	1012	271	335	9			

- Molecule 3 is a protein called Lipoprotein lipase peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			105	71	14	20			
3	D	11	Total	C	N	O	0	0	0
			105	71	14	20			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	6	Total	O	0	0
			6	6		
4	D	1	Total	O	0	0
			1	1		
4	H	6	Total	O	0	0
			6	6		

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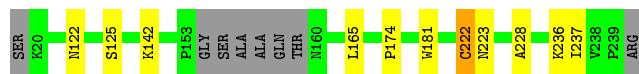
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	6	Total	O	0	0
			6	6		

### 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 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: 5D2 FAB HEAVY CHAIN

Chain A: 

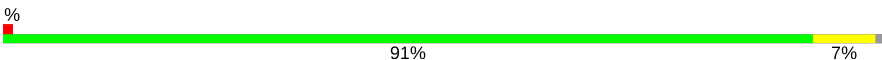


- Molecule 1: 5D2 FAB HEAVY CHAIN

Chain H: 




- Molecule 2: 5D2 FAB LIGHT CHAIN

Chain B: 




- Molecule 2: 5D2 FAB LIGHT CHAIN

Chain L: 




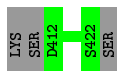
- Molecule 3: Lipoprotein lipase peptide

Chain C: 



- Molecule 3: Lipoprotein lipase peptide

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.62Å 67.75Å 130.07Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	29.26 – 2.80 29.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.26-2.80) 99.9 (29.25-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.208 , 0.243 0.217 , 0.248	Depositor DCC
$R_{free}$ test set	1066 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6822	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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	0.65	0/1707	0.74	0/2330
1	H	0.65	0/1752	0.74	0/2392
2	B	0.65	0/1632	0.74	0/2219
2	L	0.66	0/1666	0.75	0/2266
3	C	0.58	0/112	0.70	0/154
3	D	0.61	0/112	0.65	0/154
All	All	0.65	0/6981	0.74	0/9515

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	1659	0	1612	4	0
1	H	1703	0	1648	6	0
2	B	1594	0	1521	5	0
2	L	1627	0	1554	11	0
3	C	105	0	75	0	0
3	D	105	0	75	0	0
4	A	10	0	0	0	0
4	B	6	0	0	0	0
4	D	1	0	0	0	0
4	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	6	0	0	0	0
All	All	6822	0	6485	25	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 2.

All (25) 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:L:104:ALA:HB2	2:L:127:LEU:CD2	2.25	0.66
2:B:206:GLU:OE1	2:B:209:ARG:NH1	2.31	0.63
2:B:24:ILE:HD12	2:B:114:SER:HB3	1.88	0.54
1:H:180:THR:HG23	1:H:223:ASN:HB2	1.89	0.53
2:L:218:THR:HG22	2:L:225:PRO:HB3	1.92	0.52
2:L:145:GLN:HE22	2:L:152:SER:HG	1.59	0.51
2:B:207:TYR:O	2:B:213:TYR:OH	2.31	0.49
1:A:122:ASN:O	1:A:125:SER:HB2	2.13	0.48
2:L:178:ASN:N	2:L:178:ASN:OD1	2.46	0.48
1:A:165:LEU:HD22	1:A:237:ILE:HG21	1.97	0.47
2:L:104:ALA:HB2	2:L:127:LEU:HD23	1.96	0.46
2:L:207:TYR:O	2:L:213:TYR:OH	2.31	0.46
1:H:199:SER:OG	1:H:200:ASP:N	2.49	0.46
1:A:174:PRO:HD2	1:A:228:ALA:CB	2.46	0.45
2:L:129:ARG:HH12	2:L:132:ALA:HB2	1.82	0.44
1:H:212:SER:O	1:H:213:SER:CB	2.65	0.43
2:L:69:ILE:CD1	2:L:75:LEU:HD23	2.48	0.43
2:B:214:THR:HG23	2:B:227:VAL:HG13	2.00	0.43
1:H:174:PRO:HD2	1:H:228:ALA:CB	2.49	0.42
2:B:23:GLN:HA	2:B:23:GLN:OE1	2.18	0.42
2:L:205:ASP:O	2:L:209:ARG:HG3	2.19	0.41
1:H:63:GLY:HA2	2:L:108:TYR:CE1	2.56	0.41
1:H:181:TRP:CZ3	1:H:222:CYS:HB3	2.56	0.41
1:A:181:TRP:CZ3	1:A:222:CYS:HB3	2.56	0.41
2:L:145:GLN:NE2	2:L:152:SER:OG	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	210/222 (95%)	206 (98%)	4 (2%)	0	100	100
1	H	219/222 (99%)	211 (96%)	7 (3%)	1 (0%)	29	61
2	B	204/214 (95%)	194 (95%)	9 (4%)	1 (0%)	29	61
2	L	210/214 (98%)	198 (94%)	11 (5%)	1 (0%)	29	61
3	C	9/14 (64%)	9 (100%)	0	0	100	100
3	D	9/14 (64%)	9 (100%)	0	0	100	100
All	All	861/900 (96%)	827 (96%)	31 (4%)	3 (0%)	41	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	213	SER
2	B	89	GLY
2	L	89	GLY

### 5.3.2 Protein sidechains

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	188/193 (97%)	184 (98%)	4 (2%)	53	84
1	H	191/193 (99%)	185 (97%)	6 (3%)	40	74
2	B	183/188 (97%)	179 (98%)	4 (2%)	52	83
2	L	187/188 (100%)	174 (93%)	13 (7%)	15	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	11/14 (79%)	11 (100%)	0	100	100
3	D	11/14 (79%)	11 (100%)	0	100	100
All	All	771/790 (98%)	744 (96%)	27 (4%)	36	70

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LYS
1	A	222	CYS
1	A	223	ASN
1	A	236	LYS
2	B	64	SER
2	B	90	THR
2	B	148	SER
2	B	212	SER
1	H	20	LYS
1	H	132	GLN
1	H	161	SER
1	H	180	THR
1	H	222	CYS
1	H	223	ASN
2	L	24	ILE
2	L	32	LEU
2	L	34	SER
2	L	36	SER
2	L	64	SER
2	L	90	THR
2	L	129	ARG
2	L	152	SER
2	L	176	ARG
2	L	177	GLN
2	L	178	ASN
2	L	218	THR
2	L	233	ASN

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

Mol	Chain	Res	Type
1	A	22	GLN
1	H	58	GLN

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Mol	Chain	Res	Type
2	L	59	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	214/222 (96%)	-0.12	0 100 100	36, 50, 72, 87	0
1	H	221/222 (99%)	0.06	6 (2%) 54 44	41, 66, 91, 117	0
2	B	208/214 (97%)	-0.11	2 (0%) 82 77	35, 56, 82, 103	0
2	L	212/214 (99%)	0.18	4 (1%) 66 59	44, 63, 88, 102	0
3	C	11/14 (78%)	0.02	0 100 100	40, 47, 57, 66	0
3	D	11/14 (78%)	-0.02	0 100 100	43, 48, 68, 72	0
All	All	877/900 (97%)	0.00	12 (1%) 75 70	35, 60, 85, 117	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	159	THR	4.8
1	H	160	ASN	4.0
1	H	212	SER	3.5
2	L	233	ASN	3.3
2	L	174	SER	3.3
2	L	223	THR	2.9
1	H	156	ALA	2.6
2	B	219	HIS	2.2
2	L	221	THR	2.2
1	H	20	LYS	2.1
2	B	23	GLN	2.1
1	H	157	ALA	2.1

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.