



# wwPDB X-ray Structure Validation Summary Report

Apr 29, 2024 – 06:09 PM JST

PDB ID : 8YX1  
Title : CD40 in complex with Bleselumab Fab  
Authors : Caaveiro, J.M.M.; Fernandez-Perez, J.; Tsumoto, K.  
Deposited on : 2024-04-01  
Resolution : 2.70 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](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 : 2.36.2  
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) : 2.36.2

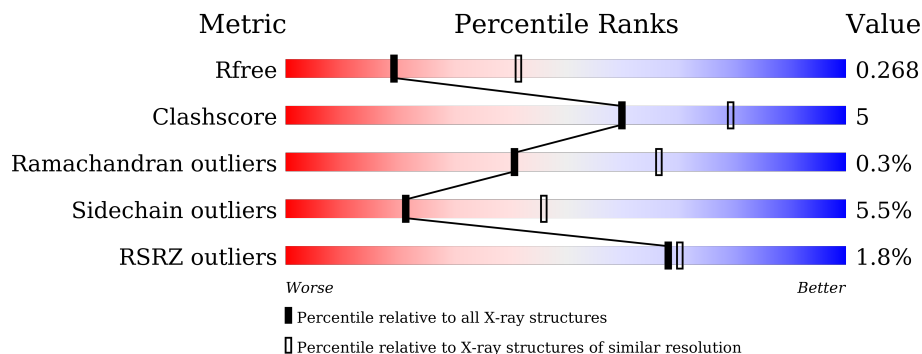
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\leq 5\%$ . 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	229	 79% 12% 6%
1	H	229	 80% 13% 6%
2	B	213	 85% 15% 2%
2	L	213	 88% 9% 2%
3	C	179	 71% 17% 11% 5%
3	R	179	 72% 12% 16% 3%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8837 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 Bleselumab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	216	Total 1612	C 1029	N 265	O 314	S 4	0	0	0
1	A	216	Total 1612	C 1029	N 265	O 314	S 4	0	0	0

- Molecule 2 is a protein called Bleselumab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	211	Total 1609	C 1007	N 270	O 328	S 4	0	0	0
2	B	211	Total 1609	C 1007	N 270	O 328	S 4	0	0	0

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	R	150	Total 1147	C 697	N 197	O 234	S 19	0	0	0
3	C	160	Total 1223	C 745	N 209	O 249	S 20	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	174	HIS	-	expression tag	UNP P25942
R	175	HIS	-	expression tag	UNP P25942
R	176	HIS	-	expression tag	UNP P25942
R	177	HIS	-	expression tag	UNP P25942
R	178	HIS	-	expression tag	UNP P25942
R	179	HIS	-	expression tag	UNP P25942
C	174	HIS	-	expression tag	UNP P25942
C	175	HIS	-	expression tag	UNP P25942

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	176	HIS	-	expression tag	UNP P25942
C	177	HIS	-	expression tag	UNP P25942
C	178	HIS	-	expression tag	UNP P25942
C	179	HIS	-	expression tag	UNP P25942

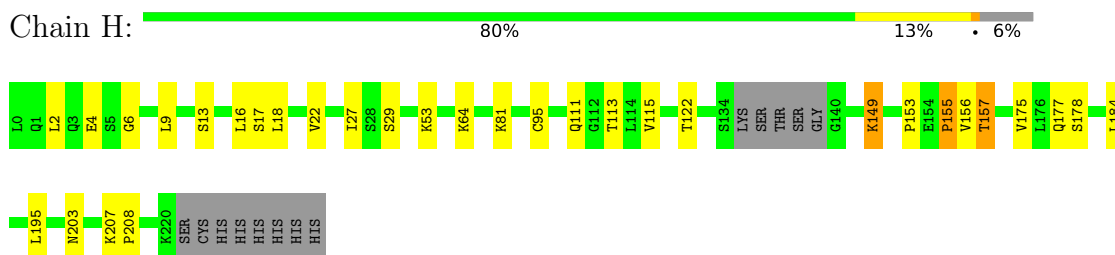
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	11	Total O 11 11	0	0
4	L	3	Total O 3 3	0	0
4	R	2	Total O 2 2	0	0
4	A	4	Total O 4 4	0	0
4	B	3	Total O 3 3	0	0
4	C	2	Total O 2 2	0	0

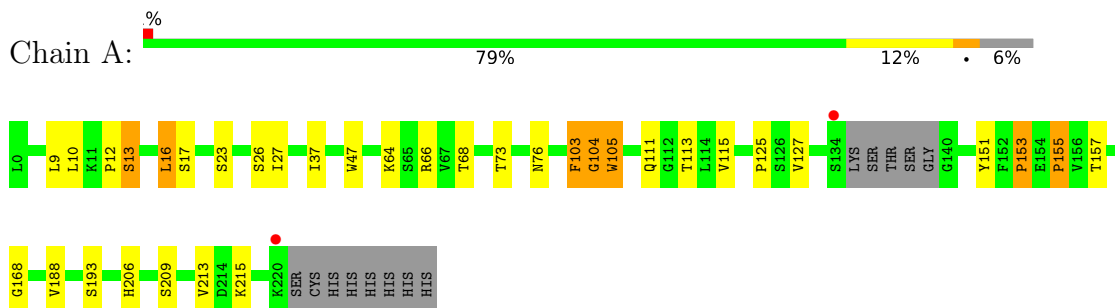
### 3 Residue-property plots [i](#)

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.

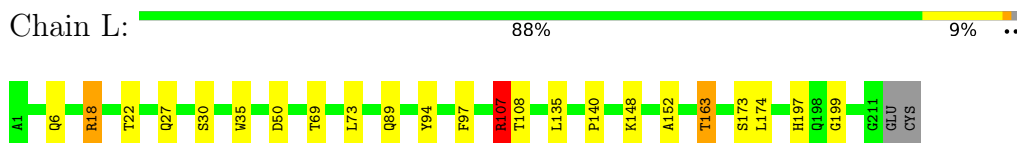
- Molecule 1: Bleselumab, heavy chain



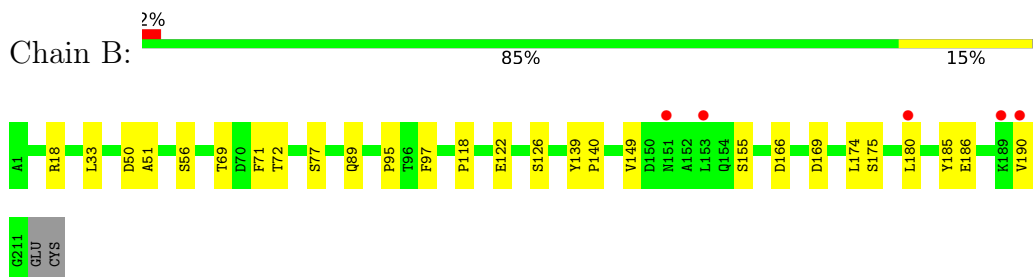
- Molecule 1: Bleselumab, heavy chain



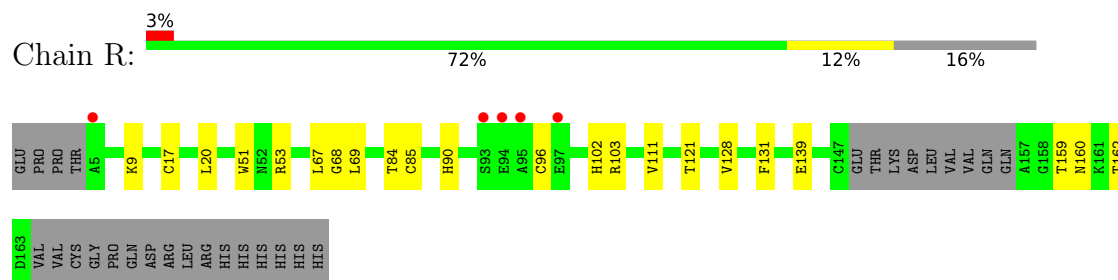
- Molecule 2: Bleselumab, light chain



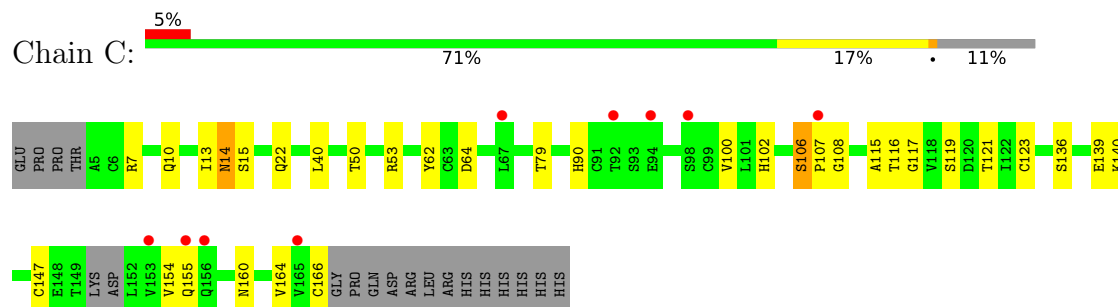
- Molecule 2: Bleselumab, light chain



- Molecule 3: Tumor necrosis factor receptor superfamily member 5



- Molecule 3: Tumor necrosis factor receptor superfamily member 5



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.56Å 116.00Å 121.65Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	45.56 – 2.70 45.56 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.56-2.70) 99.9 (45.56-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.204 , 0.265 0.209 , 0.268	Depositor DCC
$R_{free}$ test set	1858 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtrriage
Anisotropy	0.676	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 24.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k 0.016 for -h,-l,-k 0.037 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 [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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/1656	0.84	1/2263 (0.0%)
1	H	0.44	0/1656	0.85	3/2263 (0.1%)
2	B	0.40	0/1643	0.82	0/2231
2	L	0.41	0/1643	0.89	3/2231 (0.1%)
3	C	0.37	0/1248	0.84	1/1693 (0.1%)
3	R	0.42	0/1172	0.88	1/1588 (0.1%)
All	All	0.41	0/9018	0.85	9/12269 (0.1%)

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	A	0	3
2	B	0	1
2	L	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	107	ARG	NE-CZ-NH2	-8.92	115.84	120.30
2	L	27	GLN	CB-CA-C	-7.41	95.58	110.40
2	L	107	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	H	157	THR	CA-CB-OG1	-6.03	96.34	109.00
1	H	155	PRO	N-CA-CB	-5.79	96.22	102.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	103	PHE	Peptide
1	A	104	GLY	Peptide
1	A	66	ARG	Sidechain
2	L	107	ARG	Sidechain
2	L	18	ARG	Sidechain

## 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	1612	0	1601	15	0
1	H	1612	0	1601	14	0
2	B	1609	0	1567	17	0
2	L	1609	0	1567	10	0
3	C	1223	0	1117	18	0
3	R	1147	0	1038	11	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	H	11	0	0	0	0
4	L	3	0	0	0	0
4	R	2	0	0	0	0
All	All	8837	0	8491	80	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 5.

The worst 5 of 80 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:47:TRP:CE3	2:B:95:PRO:HD2	2.22	0.74
2:B:185:TYR:O	2:B:191:TYR:OH	2.13	0.67
1:A:16:LEU:HD12	1:A:115:VAL:HG11	1.77	0.65
3:C:155:GLN:H	3:C:166:CYS:HA	1.63	0.62
3:C:164:VAL:HG12	3:C:166:CYS:HB3	1.83	0.61

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	212/229 (93%)	202 (95%)	8 (4%)	2 (1%)	17	40
1	H	212/229 (93%)	200 (94%)	12 (6%)	0	100	100
2	B	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
2	L	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
3	C	156/179 (87%)	148 (95%)	7 (4%)	1 (1%)	25	50
3	R	146/179 (82%)	140 (96%)	5 (3%)	1 (1%)	22	46
All	All	1144/1242 (92%)	1087 (95%)	53 (5%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	TRP
3	R	96	CYS
1	A	13	SER
3	C	14	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	A	186/198 (94%)	173 (93%)	13 (7%)	15	35
1	H	186/198 (94%)	174 (94%)	12 (6%)	17	38
2	B	183/185 (99%)	176 (96%)	7 (4%)	33	62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	183/185 (99%)	176 (96%)	7 (4%)	33 62
3	C	145/163 (89%)	134 (92%)	11 (8%)	13 30
3	R	135/163 (83%)	129 (96%)	6 (4%)	28 56
All	All	1018/1092 (93%)	962 (94%)	56 (6%)	21 46

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
3	C	154	VAL
1	A	155	PRO
3	C	147	CYS
3	C	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	197	HIS
3	C	10	GLN
3	C	156	GLN
3	C	16	GLN
3	C	102	HIS

### 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<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	216/229 (94%)	-0.18	2 (0%) 84 85	32, 50, 80, 112	0
1	H	216/229 (94%)	-0.29	0 100 100	27, 42, 61, 102	0
2	B	211/213 (99%)	-0.12	5 (2%) 59 60	32, 48, 84, 101	0
2	L	211/213 (99%)	-0.25	0 100 100	28, 44, 67, 80	0
3	C	160/179 (89%)	0.30	9 (5%) 24 23	41, 67, 98, 114	0
3	R	150/179 (83%)	0.14	5 (3%) 46 46	37, 59, 82, 106	0
All	All	1164/1242 (93%)	-0.10	21 (1%) 68 70	27, 49, 83, 114	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	165	VAL	4.2
3	C	153	VAL	4.1
3	C	155	GLN	3.6
3	C	92	THR	3.5
2	B	153	LEU	3.4

### 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.