



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2018 – 01:51 PM EST

PDB ID : 6FAX
Title : Complex of Human CD40 Ectodomain with Lob 7.4 Fab
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Deposited on : 2017-12-18
Resolution : 2.99 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

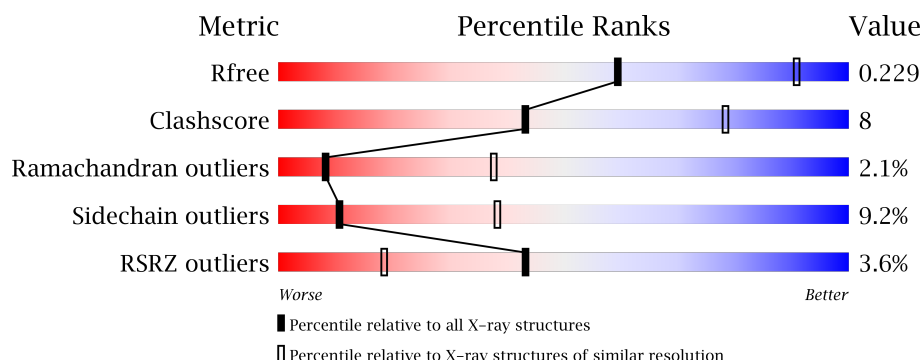
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



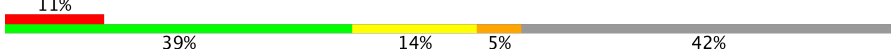
The reported resolution of this entry is 2.99 Å.

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	L	214	 76% 21% ..
2	H	240	 70% 19% 10%
3	R	173	 11% 39% 14% 5% 42%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4084 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 Lob 7.4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1629	1018	269	337	5			

- Molecule 2 is a protein called Lob 7.4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1648	1044	272	325	7			

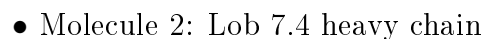
- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	100	Total	C	N	O	S	0	1	0
			786	472	134	165	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	10	Total	O	0	0
			10	10		
4	H	8	Total	O	0	0
			8	8		
4	R	3	Total	O	0	0
			3	3		

- Molecule 1: Lob 7.4 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.75Å 158.75Å 93.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	137.48 – 2.99 51.96 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (137.48-2.99) 99.7 (51.96-2.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.185 , 0.231 0.190 , 0.229	Depositor DCC
R_{free} test set	1319 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4084	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	L	0.84	0/1663	1.03	3/2261 (0.1%)
2	H	0.86	0/1688	0.99	2/2296 (0.1%)
3	R	1.03	0/802	1.18	3/1088 (0.3%)
All	All	0.89	0/4153	1.04	8/5645 (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
3	R	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	109	TRP	CA-CB-CG	7.04	127.07	113.70
2	H	187	LEU	CA-CB-CG	6.60	130.49	115.30
1	L	110	VAL	CB-CA-C	-6.51	99.04	111.40
3	R	119	CYS	CA-CB-SG	6.20	125.15	114.00
2	H	81	MET	CG-SD-CE	-6.06	90.50	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	R	106	GLU	Peptide
3	R	83	CYS	Peptide

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	L	1629	0	1573	25	0
2	H	1648	0	1620	27	0
3	R	786	0	699	16	0
4	H	8	0	0	0	0
4	L	10	0	0	1	0
4	R	3	0	0	0	0
All	All	4084	0	3892	61	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.

The worst 5 of 61 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:R:27:ARG:HB2	3:R:30:GLN:HE21	1.63	0.63
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.84	0.59
1:L:150:VAL:HG13	1:L:192:TYR:CE1	2.38	0.59
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.85	0.57
2:H:2:VAL:HG23	2:H:27:TYR:CD2	2.39	0.57

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	L	209/214 (98%)	192 (92%)	12 (6%)	5 (2%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	212/240 (88%)	197 (93%)	13 (6%)	2 (1%)	20	62
3	R	99/173 (57%)	81 (82%)	14 (14%)	4 (4%)	3	20
All	All	520/627 (83%)	470 (90%)	39 (8%)	11 (2%)	8	38

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	56	SER
1	L	157	GLY
2	H	158	PRO
3	R	64	GLU
3	R	107	GLU

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	L	188/190 (99%)	172 (92%)	16 (8%)	12	43
2	H	188/209 (90%)	172 (92%)	16 (8%)	12	43
3	R	94/157 (60%)	83 (88%)	11 (12%)	6	25
All	All	470/556 (84%)	427 (91%)	43 (9%)	11	39

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	84	ARG
2	H	159	VAL
3	R	98	GLU
2	H	91	SER
2	H	122	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	198	HIS
3	R	92	GLN
2	H	114	GLN
1	L	155	GLN
2	H	54	ASN

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 carbohydrates 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, 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(Å²)	Q<0.9	
1	L	211/214 (98%)	-0.16	0	100	100	56, 78, 108, 130	0
2	H	216/240 (90%)	-0.09	0	100	100	55, 82, 114, 148	0
3	R	100/173 (57%)	0.54	19 (19%)	1	1	62, 97, 166, 192	0
All	All	527/627 (84%)	0.00	19 (3%)	43	18	55, 82, 131, 192	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	114	GLU	3.7
3	R	109	TRP	3.6
3	R	88	GLY	3.5
3	R	84	ASP	3.5
3	R	108	GLY	3.3

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 carbohydrates 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.