



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2024 – 02:14 PM EDT

PDB ID : 8GAB
Title : Crystal structure of CTLA-4 in complex with a high affinity CTLA-4 binder
Authors : Yang, W.; Almo, S.C.; Baker, D.; Ghosh, A.
Deposited on : 2023-02-22
Resolution : 2.72 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

<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) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

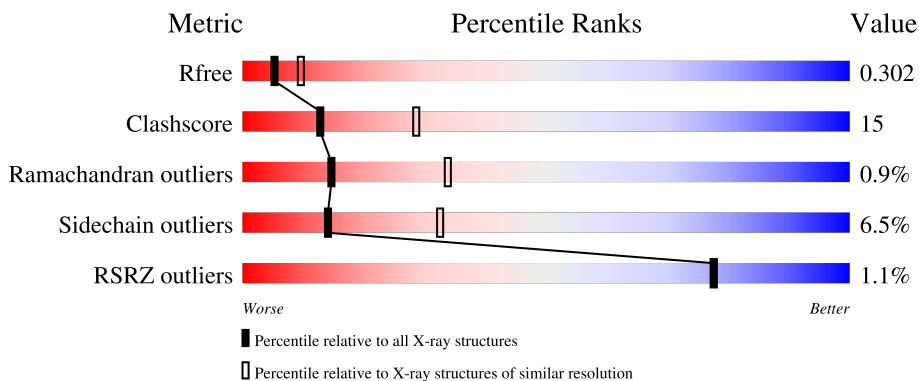
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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 ≥ 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	109	 60% 30% 6% 5%
1	C	109	 2% 70% 20% • • 6%
2	B	126	 58% 31% • 9%
2	D	126	 2% 53% 33% • • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3462 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 CTLA-4 binder.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	104	872	547	168	155	2	0	0	0
1	C	103	864	543	167	152	2	0	0	0

- Molecule 2 is a protein called Cytotoxic T-lymphocyte protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	115	860	542	141	168	9	0	0	0
2	D	115	860	542	141	168	9	0	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total 1 K 1	0	0

- Molecule 4 is water.

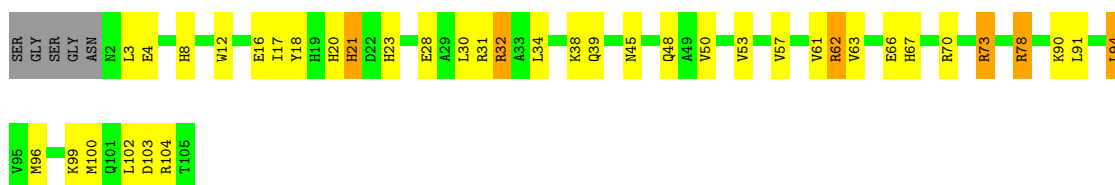
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total 2 O 2	0	0
4	C	1	Total 1 O 1	0	0
4	D	2	Total 2 O 2	0	0

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: CTLA-4 binder

Chain A: 



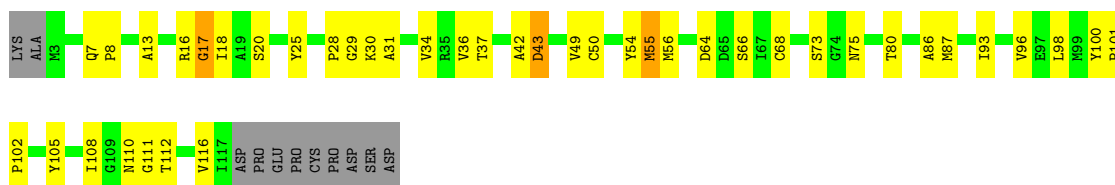
- Molecule 1: CTLA-4 binder

Chain C: 



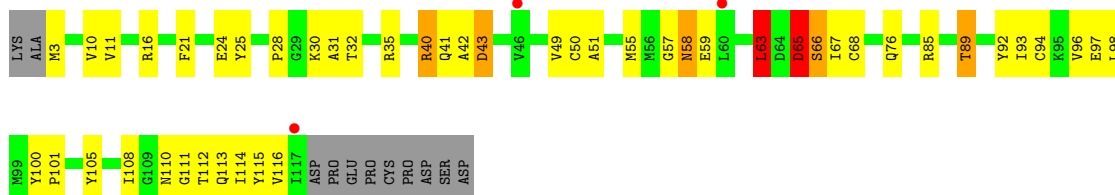
- Molecule 2: Cytotoxic T-lymphocyte protein 4

Chain B: 



- Molecule 2: Cytotoxic T-lymphocyte protein 4

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.75Å 33.60Å 74.47Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	24.95 – 2.72 24.95 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.95-2.72) 99.5 (24.95-2.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.72Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.247 , 0.292 0.247 , 0.302	Depositor DCC
R_{free} test set	550 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3462	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	1/886 (0.1%)	0.87	7/1194 (0.6%)
1	C	0.33	0/878	0.69	3/1184 (0.3%)
2	B	0.30	0/874	0.66	2/1190 (0.2%)
2	D	0.34	0/874	0.79	4/1190 (0.3%)
All	All	0.34	1/3512 (0.0%)	0.76	16/4758 (0.3%)

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
1	C	0	1
2	D	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ARG	CG-CD	-5.84	1.37	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	CG-CD-NE	-10.71	89.31	111.80
1	A	94	LEU	CB-CG-CD2	-9.35	95.10	111.00
1	A	78	ARG	CD-NE-CZ	8.96	136.14	123.60
1	A	94	LEU	CB-CG-CD1	8.04	124.66	111.00
2	D	65	ASP	CB-CG-OD2	7.78	125.30	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Peptide
1	A	32	ARG	Sidechain
1	A	78	ARG	Sidechain
1	C	73	ARG	Sidechain
2	D	65	ASP	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	A	872	0	887	36	0
1	C	864	0	880	16	0
2	B	860	0	853	37	0
2	D	860	0	853	32	0
3	D	1	0	0	0	0
4	B	2	0	0	1	0
4	C	1	0	0	1	0
4	D	2	0	0	1	0
All	All	3462	0	3473	103	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 15.

The worst 5 of 103 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:C:73:ARG:NH1	1:C:103:ASP:OD2	2.09	0.85
1:C:38:LYS:NZ	1:C:42:GLU:OE2	2.12	0.82
1:C:32:ARG:NH1	4:C:201:HOH:O	2.13	0.82
2:B:98:LEU:HD12	2:B:105:TYR:HB2	1.67	0.76
2:B:25:TYR:HH	2:B:54:TYR:HH	1.30	0.74

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	102/109 (94%)	99 (97%)	3 (3%)	0	100	100
1	C	101/109 (93%)	97 (96%)	3 (3%)	1 (1%)	13	31
2	B	113/126 (90%)	104 (92%)	8 (7%)	1 (1%)	14	34
2	D	113/126 (90%)	103 (91%)	8 (7%)	2 (2%)	7	17
All	All	429/470 (91%)	403 (94%)	22 (5%)	4 (1%)	14	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	GLY
1	C	103	ASP
2	D	66	SER
2	D	67	ILE

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	97/100 (97%)	92 (95%)	5 (5%)	19	42
1	C	96/100 (96%)	90 (94%)	6 (6%)	15	34
2	B	95/105 (90%)	91 (96%)	4 (4%)	25	51
2	D	95/105 (90%)	85 (90%)	10 (10%)	5	13
All	All	383/410 (93%)	358 (94%)	25 (6%)	14	32

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	104	ARG
2	D	41	GLN
2	D	110	ASN
2	D	40	ARG
2	D	43	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	27	HIS
2	B	76	GLN
1	C	8	HIS
1	C	21	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	104/109 (95%)	0.13	0 100 100	56, 81, 101, 121	0
1	C	103/109 (94%)	0.12	2 (1%) 66 65	50, 74, 93, 105	0
2	B	115/126 (91%)	0.19	0 100 100	60, 86, 132, 163	0
2	D	115/126 (91%)	0.47	3 (2%) 57 56	58, 96, 145, 155	0
All	All	437/470 (92%)	0.23	5 (1%) 77 77	50, 83, 134, 163	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	117	ILE	3.2
1	C	83	VAL	3.0
2	D	46	VAL	2.4
2	D	60	LEU	2.1
1	C	102	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	D	201	1/1	0.80	0.10	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.