wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 03:05 pm BST

PDB ID	:	1I85
Title	:	CRYSTAL STRUCTURE OF THE CTLA-4/B7-2 COMPLEX
Authors	:	Schwartz, J.-C.D.; Zhang, X.; Fedorov, A.A.; Nathenson, S.G.; Almo, S.C.
Deposited on	:	2001-03-12
Resolution	:	3.20 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 (i) symbol.

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

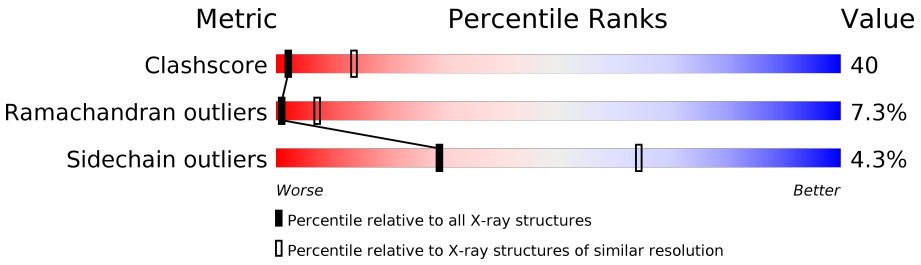
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	110	35% 55% 10%
1	B	110	35% 55% 9%
2	C	126	39% 46% 9% 6%
2	D	126	41% 42% 5% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3515 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 T LYMPHOCYTE ACTIVATION ANTIGEN CD86.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			902	572	155	169	6			
1	B	109	Total	C	N	O	S	0	0	0
			894	567	154	168	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P42081
B	0	MET	-	INITIATING METHIONINE	UNP P42081

- Molecule 2 is a protein called CYTOTOXIC T-LYMPHOCYTE-ASSOCIATED PROTEIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	118	Total	C	N	O	S	0	0	0
			882	555	144	174	9			
2	D	111	Total	C	N	O	S	0	0	0
			837	529	136	163	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	56	MET	THR	see remark 999	UNP P16410
D	56	MET	THR	see remark 999	UNP P16410

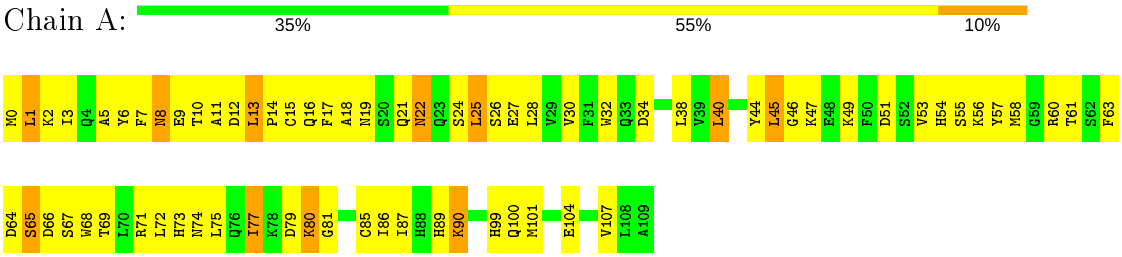
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

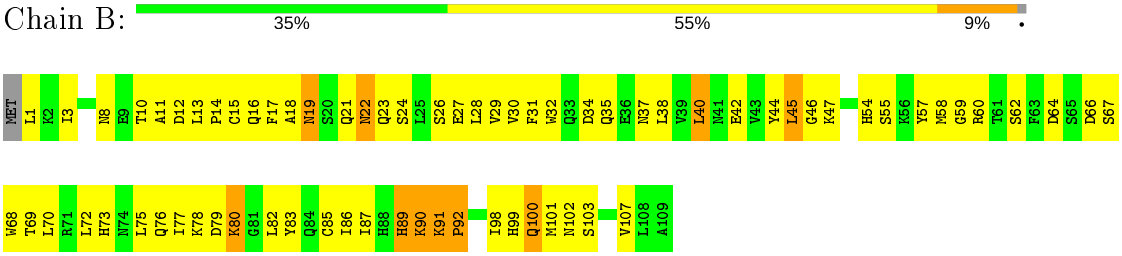
- Molecule 1: T LYMPHOCYTE ACTIVATION ANTIGEN CD86

Chain A:



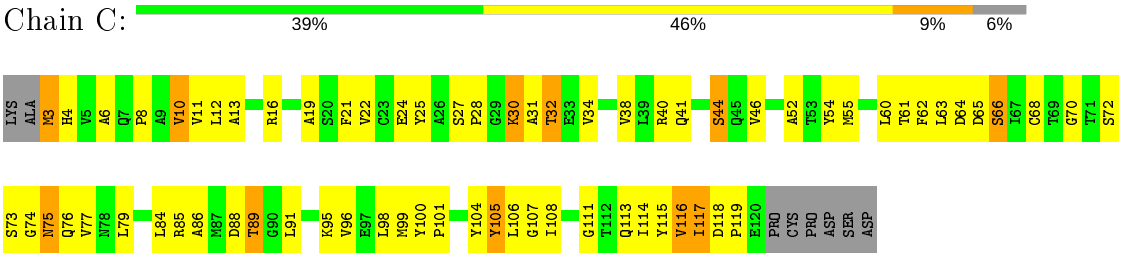
- Molecule 1: T LYMPHOCYTE ACTIVATION ANTIGEN CD86

Chain B:



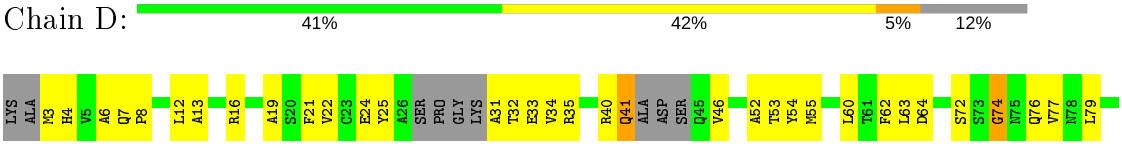
- Molecule 2: CYTOTOXIC T-LYMPHOCYTE-ASSOCIATED PROTEIN 4

Chain C:



- Molecule 2: CYTOTOXIC T-LYMPHOCYTE-ASSOCIATED PROTEIN 4

Chain D:




L84
R85
A86
M87
D88
T89
G90
L91
K95
V96
E97
L98
M99
Y100
P101
P102
P103
Y104
Y105
L106
G107
I108
G111
I114
Y115
V116
I117
D118
P119
E120
PRO
CYS
PRO
ASP
SER
ASP

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.85Å 54.56Å 103.09Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3515	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

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	0.41	0/921	0.65	0/1240
1	B	0.42	0/913	0.65	0/1230
2	C	0.45	0/897	0.75	0/1222
2	D	0.41	0/849	0.67	0/1154
All	All	0.42	0/3580	0.68	0/4846

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	902	0	886	71	0
1	B	894	0	877	86	0
2	C	882	0	865	72	0
2	D	837	0	821	60	0
All	All	3515	0	3449	276	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 40.

The worst 5 of 276 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:77:ILE:HA	1:A:80:LYS:HZ3	1.18	1.03
1:B:77:ILE:HA	1:B:80:LYS:HZ3	1.26	0.97
1:B:77:ILE:HA	1:B:80:LYS:NZ	1.80	0.95
2:C:10:VAL:HG23	2:C:113:GLN:HB3	1.50	0.94
2:C:13:ALA:HB3	2:C:116:VAL:HG13	1.50	0.92

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	108/110 (98%)	83 (77%)	18 (17%)	7 (6%)	1 10
1	B	107/110 (97%)	77 (72%)	23 (22%)	7 (6%)	1 10
2	C	116/126 (92%)	91 (78%)	14 (12%)	11 (10%)	0 3
2	D	105/126 (83%)	80 (76%)	18 (17%)	7 (7%)	1 9
All	All	436/472 (92%)	331 (76%)	73 (17%)	32 (7%)	1 7

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	22	ASN
1	A	45	LEU
1	B	22	ASN
1	B	45	LEU

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	102/102 (100%)	97 (95%)	5 (5%)	25	61
1	B	101/102 (99%)	97 (96%)	4 (4%)	31	66
2	C	97/105 (92%)	92 (95%)	5 (5%)	23	59
2	D	92/105 (88%)	89 (97%)	3 (3%)	38	71
All	All	392/414 (95%)	375 (96%)	17 (4%)	29	64

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	89	HIS
1	B	100	GLN
2	C	116	VAL
1	B	40	LEU
2	D	16	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	HIS
1	B	74	ASN
2	C	45	GLN
1	B	37	ASN
2	C	76	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.