wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 05:05 PM EDT

PDB ID	:	1WIQ
Title	:	STRUCTURE OF T-CELL SURFACE GLYCOPROTEIN CD4, TRIGONAL CRYSTAL FORM
Authors	:	Wu, H.; Kwong, P.D.; Hendrickson, W.A.
Deposited on	:	1996-12-18
Resolution	:	5.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

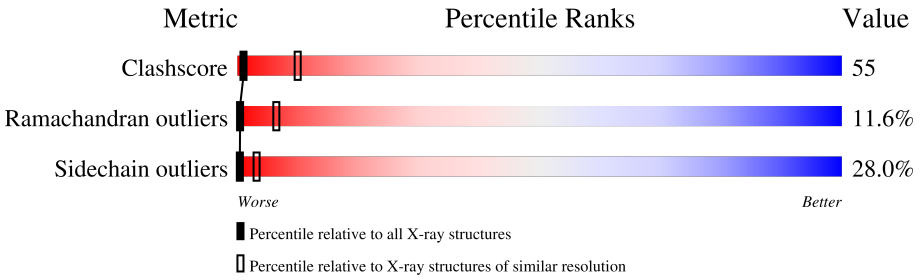
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 5.00 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	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	22% 52% 21% .
1	B	363	25% 50% 22% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5624 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-CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2812	1784	479	539	10			
1	B	363	Total	C	N	O	S	0	0	0
			2812	1784	479	539	10			

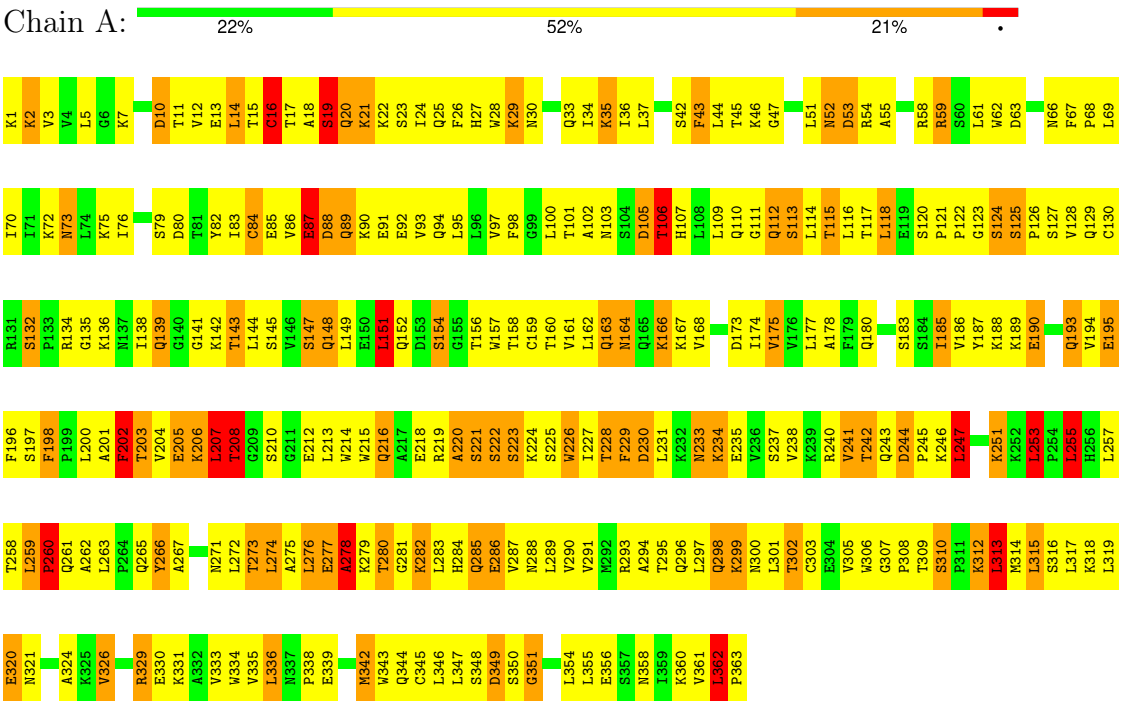
3 Residue-property plots (i)

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. 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.

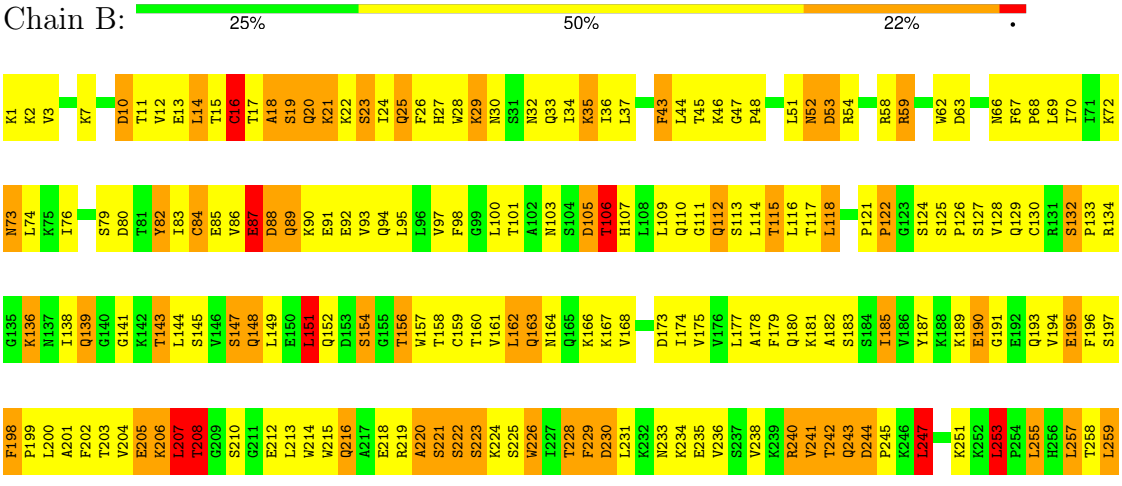
• Molecule 1: T-CELL SURFACE GLYCOPROTEIN CD4

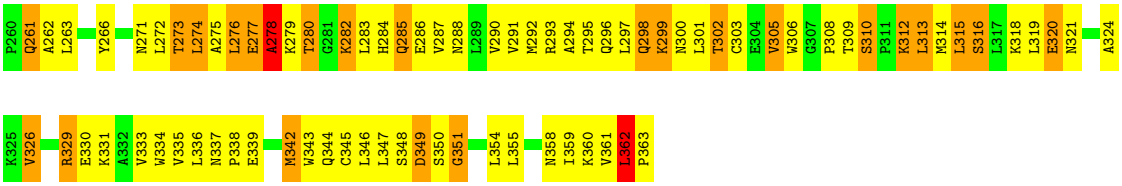
Chain A:



• Molecule 1: T-CELL SURFACE GLYCOPROTEIN CD4

Chain B:




P260
Q261
A262
L263
Y266
M271
L272
T273
L274
A275
L276
E277
A278
K279
T280
G281
K282
L283
H284
Q285
E286
V287
N288
L289
V290
V291
M292
R293
A294
T295
Q296
L297
Q298
K299
N300
L301
T302
C303
E304
V305
W306
G307
P308
T309
S310
P311
K312
L313
M314
L315
S316
L317
K318
L319
E320
N321
A324
K325
V326
R329
E330
K331
A332
V333
W334
V335
L336
N337
P338
E339
M342
W343
Q344
C345
L346
L347
S348
D349
S350
G351
L354
L355
N358
I359
K360
V361
L362
P363

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.00Å 126.00Å 205.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 5.00	Depositor
% Data completeness (in resolution range)	67.3 (8.00-5.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.422 , 0.442	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5624	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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	0.72	1/2860 (0.0%)	1.04	13/3868 (0.3%)
1	B	0.66	0/2860	1.01	9/3868 (0.2%)
All	All	0.69	1/5720 (0.0%)	1.03	22/7736 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	PHE	C-O	-5.14	1.13	1.23

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	THR	N-CA-C	8.38	133.62	111.00
1	A	208	THR	N-CA-C	7.55	131.40	111.00
1	B	277	GLU	O-C-N	6.99	133.88	122.70
1	A	277	GLU	O-C-N	6.97	133.86	122.70
1	B	247	LEU	CA-CB-CG	6.89	131.14	115.30

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	2812	0	2872	330	29
1	B	2812	0	2870	301	32
All	All	5624	0	5742	620	32

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 55.

The worst 5 of 620 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:B:151:LEU:CD2	1:B:180:GLN:HA	1.55	1.33
1:B:177:LEU:HD13	1:B:283:LEU:CD1	1.60	1.31
1:B:151:LEU:HD21	1:B:180:GLN:CA	1.63	1.28
1:B:178:ALA:CB	1:B:179:PHE:O	1.86	1.19
1:A:109:LEU:HD13	1:A:280:THR:O	1.47	1.13

The worst 5 of 32 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:SER:CA	1:B:362:LEU:CD1[3_664]	0.99	1.21
1:A:124:SER:N	1:B:362:LEU:CD1[3_664]	1.08	1.12
1:A:142:LYS:CB	1:B:297:LEU:O[3_664]	1.13	1.07
1:A:123:GLY:CA	1:B:362:LEU:CD2[3_664]	1.24	0.96
1:A:123:GLY:O	1:B:362:LEU:CB[3_664]	1.24	0.96

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	359/363 (99%)	259 (72%)	58 (16%)	42 (12%)	0 6
1	B	359/363 (99%)	259 (72%)	59 (16%)	41 (11%)	0 7
All	All	718/726 (99%)	518 (72%)	117 (16%)	83 (12%)	0 6

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	52	ASN
1	A	73	ASN
1	A	87	GLU
1	A	88	ASP

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	318/324 (98%)	227 (71%)	91 (29%)	0 3
1	B	318/324 (98%)	231 (73%)	87 (27%)	0 3
All	All	636/648 (98%)	458 (72%)	178 (28%)	0 3

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	SER
1	B	223	SER
1	B	139	GLN
1	B	166	LYS
1	B	238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	GLN
1	B	261	GLN
1	B	288	ASN
1	B	284	HIS
1	A	193	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	178:ALA	C	179:PHE	N	2.89
1	B	178:ALA	C	179:PHE	N	2.73

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.