



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:27 PM GMT

PDB ID : 5DFW
Title : CRYSTAL STRUCTURE OF HUMAN CD81 LARGE EXTRACELLULAR
LOOP IN COMPLEX WITH SINGLE CHAIN FV FRAGMENT K13
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Deposited on : 2015-08-27
Resolution : 2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

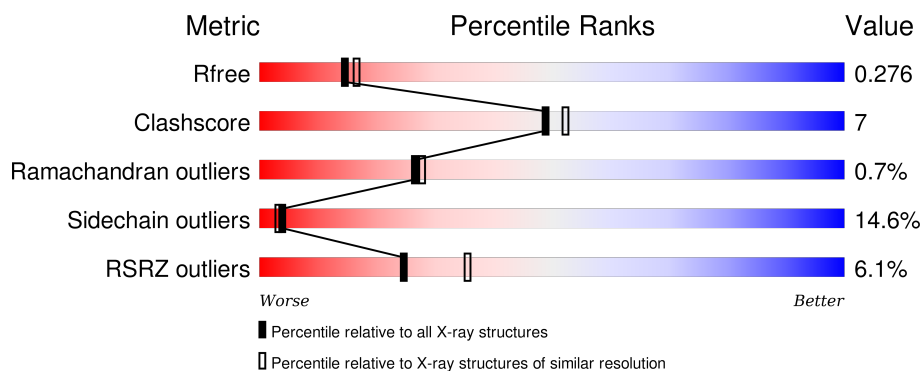
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	A	98	<div> <div> <div>7%</div> <div>69%</div> <div>21%</div> <div>8%</div> </div> </div>
2	H	243	<div> <div>7%</div> <div>65%</div> <div>23%</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2501 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 CD81 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			693	430	118	141	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLY	-	expression tag	UNP P60033
A	111	SER	-	expression tag	UNP P60033
A	202	HIS	-	expression tag	UNP P60033
A	203	HIS	-	expression tag	UNP P60033
A	204	HIS	-	expression tag	UNP P60033
A	205	HIS	-	expression tag	UNP P60033
A	206	HIS	-	expression tag	UNP P60033
A	207	HIS	-	expression tag	UNP P60033

- Molecule 2 is a protein called SINGLE CHAIN FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1725	1095	291	333	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	H	55	Total	O	0	0
			55	55		

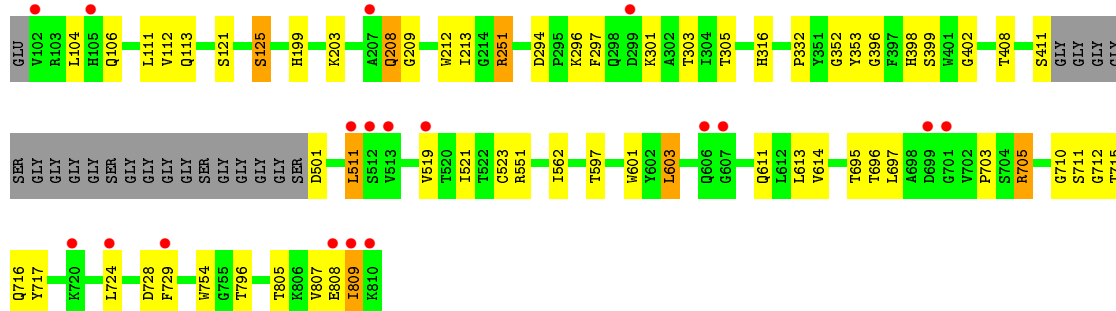
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CD81 antigen



- Molecule 2: SINGLE CHAIN FV FRAGMENT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	49.65Å 49.67Å 80.45Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	41.83 – 2.33 38.80 – 2.33	Depositor EDS
% Data completeness (in resolution range)	68.2 (41.83-2.33) 68.3 (38.80-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.190 , 0.264 0.194 , 0.276	Depositor DCC
R_{free} test set	577 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.5	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 11218 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2501	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.51	0/702	0.72	0/948
2	H	0.47	0/1771	0.74	0/2410
All	All	0.48	0/2473	0.74	0/3358

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	693	0	672	9	0
2	H	1725	0	1652	29	0
3	A	28	0	0	0	0
3	H	55	0	0	3	0
All	All	2501	0	2324	34	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 7.

All (34) 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:173:ASN:HD21	2:H:396:GLY:H	1.22	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:HIS:HD2	2:H:212:TRP:HE1	1.23	0.84
2:H:104:LEU:HD21	2:H:332:PRO:HD3	1.63	0.79
2:H:398:HIS:NE2	3:H:901:HOH:O	2.21	0.74
2:H:199:HIS:CD2	2:H:212:TRP:HE1	2.12	0.63
2:H:353:TYR:N	3:H:901:HOH:O	2.32	0.63
2:H:303:THR:HB	2:H:316:HIS:HB2	1.83	0.60
2:H:203:LYS:HB2	2:H:213:ILE:HD11	1.83	0.59
2:H:521:ILE:HG12	2:H:805:THR:HG21	1.86	0.57
2:H:603:LEU:HB2	2:H:613:LEU:HD11	1.84	0.57
2:H:562:ILE:O	2:H:597:THR:HG22	2.06	0.56
1:A:201:LYS:O	1:A:202:HIS:ND1	2.42	0.51
2:H:104:LEU:H	2:H:104:LEU:HD12	1.76	0.49
2:H:305:THR:OG1	2:H:316:HIS:HE1	1.96	0.48
1:A:184:ASN:HD22	1:A:187:LYS:HD2	1.79	0.47
2:H:601:TRP:HD1	2:H:614:VAL:HG22	1.79	0.47
2:H:597:THR:HG21	2:H:754:TRP:HE3	1.80	0.47
2:H:352:GLY:N	3:H:901:HOH:O	2.47	0.46
1:A:170:LEU:O	2:H:352:GLY:O	2.33	0.46
2:H:106:GLN:HE21	2:H:402:GLY:HA3	1.80	0.46
2:H:551:ARG:HG3	2:H:716:GLN:HG2	1.98	0.45
2:H:703:PRO:HB2	2:H:705:ARG:HG2	1.98	0.45
2:H:710:GLY:HA3	2:H:717:TYR:HA	1.98	0.45
2:H:199:HIS:CD2	2:H:251:ARG:HB2	2.52	0.44
1:A:196:ASP:HB3	1:A:201:LYS:O	2.18	0.44
2:H:208:GLN:HE21	2:H:209:GLY:H	1.65	0.43
1:A:171:LYS:O	2:H:352:GLY:HA2	2.18	0.43
2:H:523:CYS:HB2	2:H:601:TRP:CH2	2.53	0.43
1:A:135:VAL:HG21	1:A:165:LEU:HD22	1.99	0.43
2:H:511:LEU:HB3	2:H:807:VAL:HG12	2.01	0.43
1:A:173:ASN:ND2	2:H:352:GLY:O	2.52	0.42
2:H:729:PHE:CZ	2:H:809:ILE:HG23	2.54	0.42
2:H:294:ASP:HB3	2:H:297:PHE:HD1	1.85	0.42
1:A:131:LEU:HD11	1:A:169:VAL:HG22	2.01	0.41

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	A	88/98 (90%)	86 (98%)	2 (2%)	0	100	100
2	H	218/243 (90%)	206 (94%)	10 (5%)	2 (1%)	21	21
All	All	306/341 (90%)	292 (95%)	12 (4%)	2 (1%)	26	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	712	GLY
2	H	125	SER

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	A	80/86 (93%)	69 (86%)	11 (14%)	4	4
2	H	188/193 (97%)	160 (85%)	28 (15%)	4	3
All	All	268/279 (96%)	229 (85%)	39 (15%)	4	3

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	147	VAL
1	A	148	LYS
1	A	161	THR

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Mol	Chain	Res	Type
1	A	163	THR
1	A	168	SER
1	A	181	ILE
1	A	185	LEU
1	A	189	ASP
1	A	193	LYS
1	A	202	HIS
2	H	111	LEU
2	H	112	VAL
2	H	113	GLN
2	H	121	SER
2	H	125	SER
2	H	208	GLN
2	H	251	ARG
2	H	296	LYS
2	H	301	LYS
2	H	399	SER
2	H	408	THR
2	H	411	SER
2	H	501	ASP
2	H	511	LEU
2	H	519	VAL
2	H	603	LEU
2	H	611	GLN
2	H	695	THR
2	H	696	THR
2	H	697	LEU
2	H	705	ARG
2	H	711	SER
2	H	715	THR
2	H	724	LEU
2	H	728	ASP
2	H	796	THR
2	H	808	GLU
2	H	809	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	129	GLN
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	184	ASN
2	H	106	GLN
2	H	199	HIS
2	H	208	GLN
2	H	316	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 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(Å ²)	Q<0.9
1	A	90/98 (91%)	0.04	1 (1%) 82 89	23, 36, 54, 67	0
2	H	222/243 (91%)	0.51	18 (8%) 15 23	24, 49, 75, 107	0
All	All	312/341 (91%)	0.37	19 (6%) 25 35	23, 45, 73, 107	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	102	VAL	8.7
2	H	729	PHE	4.9
2	H	809	ILE	3.9
2	H	513	VAL	3.9
2	H	810	LYS	3.9
2	H	808	GLU	3.3
2	H	105	HIS	3.3
2	H	512	SER	3.0
2	H	519	VAL	3.0
2	H	701	GLY	2.6
2	H	511	LEU	2.5
2	H	699	ASP	2.4
2	H	607	GLY	2.4
1	A	160	SER	2.4
2	H	207	ALA	2.3
2	H	720	LYS	2.3
2	H	606	GLN	2.3
2	H	299	ASP	2.2
2	H	724	LEU	2.1

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.