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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2020 – 10:40 pm BST

PDB ID	:	1IKF
Title	:	A CONFORMATION OF CYCLOSPORIN A IN AQUEOUS ENVIRON-MENT REVEALED BY THE X-RAY STRUCTURE OF A CYCLOSPORIN-FAB COMPLEX
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Deposited on	:	1993-12-09
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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 2.50 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.
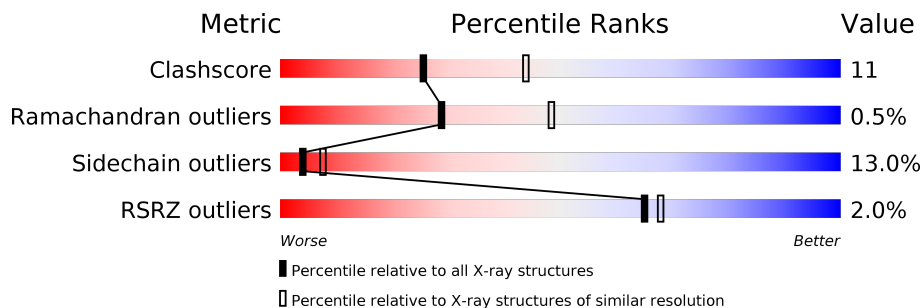
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	65% 30%
2	H	228	65% 29% 5%
3	C	11	27% 73%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3651 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 IGG1-KAPPA R45-45-11 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1652	1024	281	340	7			

- Molecule 2 is a protein called IGG1-KAPPA R45-45-11 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1742	1107	288	338	9			

- Molecule 3 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			85	62	11	12			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	96	Total	O	0	0
			96	96		
4	H	69	Total	O	0	0
			69	69		
4	C	7	Total	O	0	0
			7	7		

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 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: IGG1-KAPPA R45-45-11 FAB (LIGHT CHAIN)
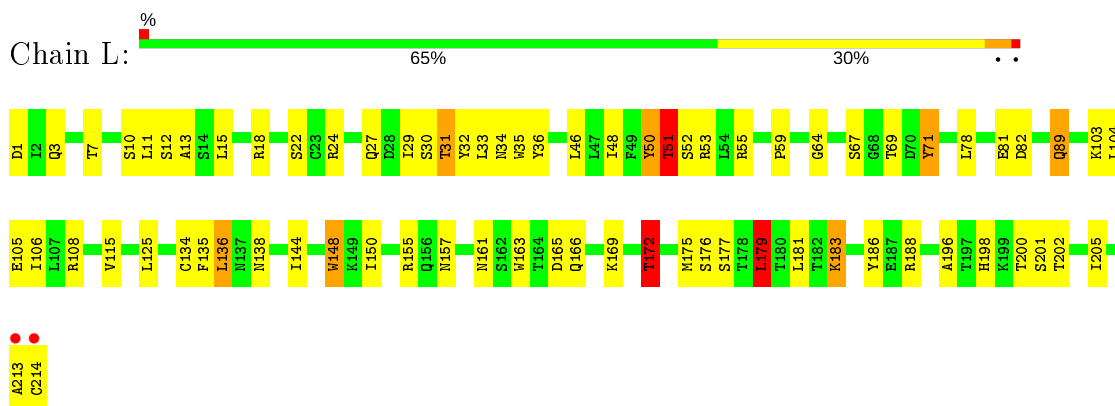
• Molecule 2: IGG1-KAPPA R45-45-11 FAB (HEAVY CHAIN)
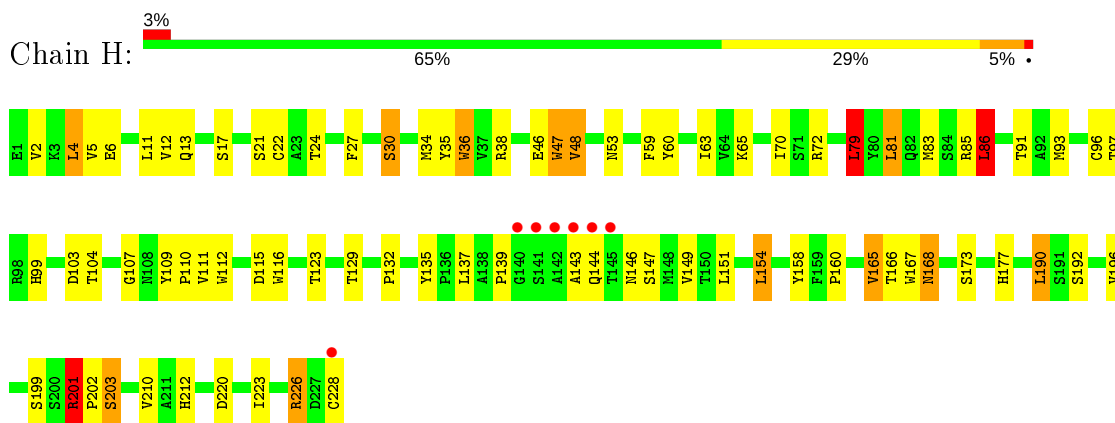
• Molecule 3: CYCLOSPORIN A

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	52.60Å 70.20Å 118.40Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	8.00 – 2.50	Depositor
	17.36 – 2.39	EDS
% Data completeness	(Not available) (8.00-2.50)	Depositor
(in resolution range)	78.3 (17.36-2.39)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.164 , (Not available)	Depositor
	0.170 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 66.1	EDS
L-test for twinning[1]	$<|L|> = 0.44, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3651	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical values of $<|L|>$, $<L^2>$ 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: ABA, MLE, DAL, MVA, BMT, SAR

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	0.86	0/1685	1.67	30/2286 (1.3%)
2	H	0.89	0/1788	1.76	36/2439 (1.5%)
3	C	1.05	0/10	2.04	0/11
All	All	0.88	0/3483	1.72	66/4736 (1.4%)

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
2	H	0	1

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	201	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	L	148	TRP	CD1-CG-CD2	10.73	114.88	106.30
1	L	32	TYR	CB-CG-CD2	-10.56	114.66	121.00
2	H	48	VAL	CG1-CB-CG2	-10.25	94.50	110.90
2	H	36	TRP	CD1-CG-CD2	8.88	113.40	106.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	35	TYR	Sidechain

5.2 Too-close contacts (i)

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	1652	0	1594	33	0
2	H	1742	0	1699	35	0
3	C	85	0	109	8	0
4	C	7	0	0	0	0
4	H	69	0	0	0	0
4	L	96	0	0	4	0
All	All	3651	0	3402	73	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 11.

The worst 5 of 73 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)
2:H:201:ARG:HG2	2:H:202:PRO:HA	1.66	0.77
1:L:106:ILE:H	1:L:166:GLN:HE22	1.36	0.73
2:H:53:ASN:HA	2:H:72:ARG:NH1	2.03	0.73
2:H:201:ARG:HH11	2:H:201:ARG:HB3	1.55	0.70
1:L:138:ASN:HD22	1:L:172:THR:HG21	1.61	0.66

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	L	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	29	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	226/228 (99%)	217 (96%)	8 (4%)	1 (0%)	34	54
3	C	1/11 (9%)	1 (100%)	0	0	100	100
All	All	439/453 (97%)	417 (95%)	20 (5%)	2 (0%)	29	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	51	THR
2	H	143	ALA

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	L	190/190 (100%)	166 (87%)	24 (13%)	4	8
2	H	195/195 (100%)	169 (87%)	26 (13%)	4	7
3	C	1/1 (100%)	1 (100%)	0	100	100
All	All	386/386 (100%)	336 (87%)	50 (13%)	4	7

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	202	THR
2	H	30	SER
2	H	210	VAL
1	L	214	CYS
2	H	13	GLN

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	161	ASN
2	H	212	HIS

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Mol	Chain	Res	Type
1	L	198	HIS
1	L	157	ASN
1	L	166	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)

9 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	MLE	C	502	3	7,8,9	0.83	0	6,9,11	1.32	1 (16%)
3	BMT	C	505	3	11,12,13	1.88	3 (27%)	12,14,16	2.00	3 (25%)
3	SAR	C	507	3	4,4,5	0.98	0	1,3,5	0.88	0
3	MLE	C	508	3	7,8,9	0.78	0	6,9,11	1.26	1 (16%)
3	MLE	C	510	3	7,8,9	0.80	0	6,9,11	1.27	1 (16%)
3	MVA	C	504	3	6,7,8	0.82	0	7,8,10	1.89	1 (14%)
3	ABA	C	506	3	4,5,6	0.62	0	1,5,7	2.72	1 (100%)
3	MLE	C	503	3	7,8,9	0.75	0	6,9,11	1.36	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLE	C	502	3	-	2/5/8/10	-
3	BMT	C	505	3	-	4/13/16/18	-
3	SAR	C	507	3	-	1/1/2/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLE	C	508	3	-	3/5/8/10	-
3	MLE	C	510	3	-	0/5/8/10	-
3	MVA	C	504	3	-	4/6/8/10	-
3	ABA	C	506	3	-	0/3/4/6	-
3	MLE	C	503	3	-	3/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	505	BMT	CE-CZ	3.55	1.56	1.29
3	C	505	BMT	CG2-CB	3.37	1.59	1.53
3	C	505	BMT	CA-N	-2.35	1.43	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	504	MVA	CB-CA-C	-3.89	108.17	113.04
3	C	505	BMT	O-C-CA	-3.73	114.44	124.83
3	C	505	BMT	CG2-CD2-CE	3.17	118.86	113.98
3	C	505	BMT	CD1-CG2-CD2	-3.01	105.49	110.54
3	C	506	ABA	CG-CB-CA	2.72	119.65	113.42

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	MLE	C-CA-CB-CG
3	C	505	BMT	CE-CD2-CG2-CB
3	C	505	BMT	CE-CD2-CG2-CD1
3	C	505	BMT	CD2-CE-CZ-CH
3	C	507	SAR	C-CA-N-CN

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	MLE	2	0
3	C	505	BMT	1	0
3	C	508	MLE	1	0
3	C	510	MLE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	MVA	2	0
3	C	503	MLE	3	0

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	L	214/214 (100%)	-0.84	2 (0%)	84	86	2, 7, 26, 59	0
2	H	228/228 (100%)	-0.71	7 (3%)	49	52	2, 8, 32, 58	0
3	C	2/11 (18%)	-0.76	0	100	100	18, 18, 18, 30	0
All	All	444/453 (98%)	-0.77	9 (2%)	65	68	2, 8, 30, 59	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	214	CYS	5.6
2	H	143	ALA	5.4
2	H	145	THR	3.4
1	L	213	ALA	2.9
2	H	142	ALA	2.8

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
3	BMT	C	505	13/14	0.89	0.17	5,13,19,19	0
3	MLE	C	503	9/10	0.90	0.14	13,16,19,20	0
3	DAL	C	501	5/6	0.91	0.16	25,25,28,28	0
3	MLE	C	502	9/10	0.91	0.17	18,19,22,23	0
3	MLE	C	510	9/10	0.93	0.10	16,21,25,25	0
3	MVA	C	504	8/9	0.95	0.15	2,9,12,14	0
3	MLE	C	508	9/10	0.96	0.10	7,15,19,21	0
3	ABA	C	506	6/7	0.97	0.09	5,7,8,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SAR	C	507	5/6	0.97	0.10	10,14,15,17	0

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.