



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:00 PM GMT

PDB ID : 1RMH
Title : RECOMBINANT CYCLOPHILIN A FROM HUMAN T CELL
Authors : Zhao, Y.; Ke, H.
Deposited on : 1995-07-31
Resolution : 2.40 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

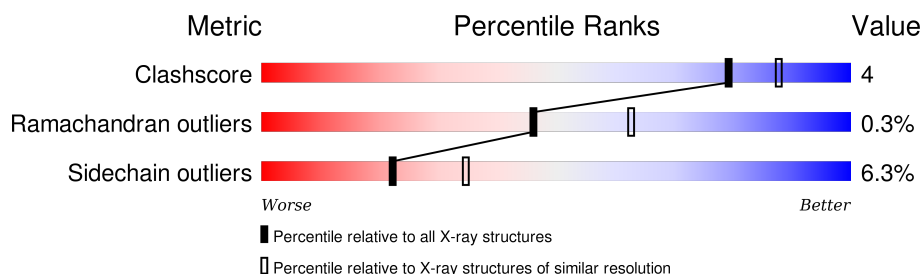
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	<div> <div style="width: 84%;"></div> <div style="width: 14%;"></div> <div style="width: 2%;"></div> </div> <div>84% 14% .</div>
1	B	164	<div> <div style="width: 82%;"></div> <div style="width: 13%;"></div> <div style="width: 5%;"></div> </div> <div>82% 13% 5%</div>
2	C	6	<div> <div style="width: 100%;"></div> </div> <div>100%</div>
2	D	6	<div> <div style="width: 100%;"></div> </div> <div>100%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3300 atoms, of which 656 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 CYCLOPHILIN A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total	C	H	N	O	S	0	0	0
			1544	797	286	217	236	8			
1	B	164	Total	C	H	N	O	S	0	0	0
			1544	797	286	217	236	8			

- Molecule 2 is a protein called AAPF PEPTIDE SUBSTRATE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	H	N	O	0	0	0
			49	30	4	6	9			
2	D	6	Total	C	H	N	O	0	0	0
			49	30	4	6	9			

- Molecule 3 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	15	Total	H	O	0	0
			45	30	15		
3	B	23	Total	H	O	0	0
			69	46	23		

3 Residue-property plots

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.


Note EDS was not executed.

- Molecule 1: CYCLOPHILIN A

Chain A: 



- Molecule 1: CYCLOPHILIN A

Chain B: 



- Molecule 2: AAPF PEPTIDE SUBSTRATE

Chain C: 

There are no outlier residues recorded for this chain.

- Molecule 2: AAPF PEPTIDE SUBSTRATE

Chain D: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	37.80 Å 109.20 Å 118.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3300	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.84	0/1286	1.45	11/1723 (0.6%)
1	B	0.80	0/1286	1.44	9/1723 (0.5%)
2	C	0.92	0/29	1.53	0/39
2	D	0.90	0/29	1.40	0/39
All	All	0.82	0/2630	1.44	20/3524 (0.6%)

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	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	121	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	B	121	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	121	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	148	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	55	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	121	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	B	61	MET	CA-CB-CG	6.29	123.99	113.30
1	B	19	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	31	LYS	N-CA-CB	-5.62	100.48	110.60
1	A	55	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	34	GLU	OE1-CD-OE2	-5.51	116.68	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	CYS	CA-CB-SG	5.24	123.44	114.00
1	B	48	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	A	37	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	148	ARG	CA-CB-CG	5.15	124.72	113.40
1	B	116	THR	CA-CB-CG2	-5.10	105.26	112.40
1	A	31	LYS	CA-CB-CG	5.05	124.50	113.40
1	A	134	GLU	OE1-CD-OE2	-5.01	117.28	123.30
1	A	8	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	PHE	Sidechain

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	1258	286	1225	8	1
1	B	1258	286	1225	12	1
2	C	45	4	33	0	0
2	D	45	4	34	0	0
3	A	15	30	0	0	0
3	B	23	46	0	0	0
All	All	2644	656	2517	18	1

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 4.

All (18) 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:5:THR:HB	1:A:165:GLU:HG2	1.65	0.78
1:B:5:THR:HB	1:B:165:GLU:HG2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:TRP:HZ3	1:B:148:ARG:NH2	2.05	0.55
1:A:121:TRP:HZ3	1:B:148:ARG:HH22	1.57	0.53
1:A:91:LYS:HZ3	1:A:123:ASP:HB3	1.78	0.47
1:A:121:TRP:O	1:A:125:LYS:NZ	2.47	0.47
1:B:82:LYS:HD2	1:B:107:THR:HA	1.96	0.47
1:B:141:ALA:O	1:B:144:ARG:HB3	2.15	0.46
1:A:100:MET:HG2	1:A:129:PHE:CE1	2.52	0.45
1:A:27:ASP:OD2	1:A:28:LYS:NZ	2.50	0.44
1:B:121:TRP:O	1:B:125:LYS:NZ	2.52	0.42
1:B:147:SER:OG	1:B:151:LYS:HD3	2.19	0.41
1:B:118:LYS:HZ3	1:B:120:GLU:HB3	1.85	0.41
1:B:5:THR:HA	1:B:22:PHE:O	2.20	0.41
1:B:27:ASP:OD2	1:B:28:LYS:NZ	2.53	0.41
1:B:99:SER:HB3	1:B:113:PHE:CZ	2.55	0.41
1:A:82:LYS:HA	1:A:108:ASN:O	2.21	0.40
1:B:145:PHE:O	1:B:152:THR:HA	2.22	0.40

All (1) 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:154:LYS:HZ3	1:B:140:GLU:OE1[4_566]	1.29	0.31

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	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	B	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	30	43
2	C	2/6 (33%)	2 (100%)	0	0	100	100
2	D	2/6 (33%)	2 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	328/340 (96%)	306 (93%)	21 (6%)	1 (0%)	46 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	81	GLU

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	132/132 (100%)	123 (93%)	9 (7%)	20 31
1	B	132/132 (100%)	124 (94%)	8 (6%)	23 36
2	C	2/2 (100%)	2 (100%)	0	100 100
2	D	2/2 (100%)	2 (100%)	0	100 100
All	All	268/268 (100%)	251 (94%)	17 (6%)	22 35

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	61	MET
1	A	84	GLU
1	A	91	LYS
1	A	120	GLU
1	A	134	GLU
1	A	144	ARG
1	A	151	LYS
1	A	165	GLU
1	B	21	SER
1	B	29	VAL
1	B	61	MET
1	B	81	GLU
1	B	82	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	GLU
1	B	147	SER
1	B	151	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.