wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 09:08 PM EDT

PDB ID	:	1CD1
Title	:	CD1(MOUSE) ANTIGEN PRESENTING MOLECULE
Authors	:	Zeng, Z.H.; Segelke, B.W.; Wilson, I.A.
Deposited on	:	1997-04-02
Resolution	:	2.67 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:

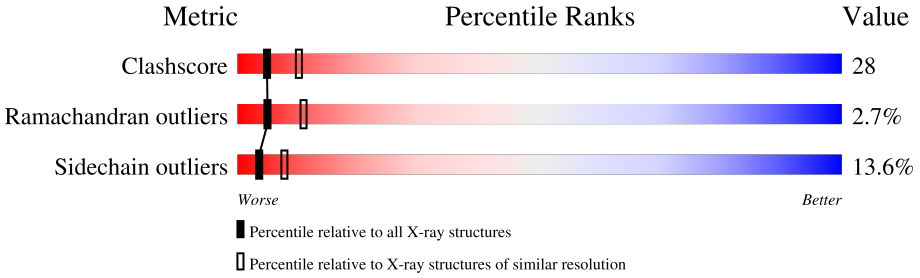
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.67 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	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)

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	315	37% 38% 10% • 13%
1	C	315	36% 36% 13% • 13%
2	B	99	46% 41% 10% •
2	D	99	46% 40% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6026 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 CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2192	1396	378	405	13	0	0	0
1	C	273	2192	1396	378	405	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	conflict	UNP P11609
C	201	HIS	ASP	conflict	UNP P11609

- Molecule 2 is a protein called CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	821	524	138	152	7	0	0	0
2	D	99	821	524	138	152	7	0	0	0

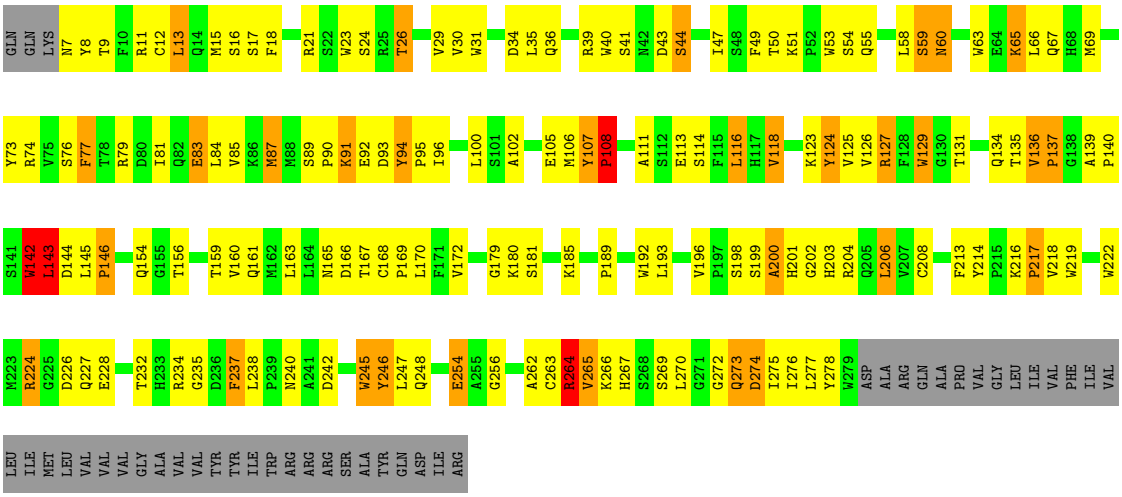
3 Residue-property plots (i)

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.

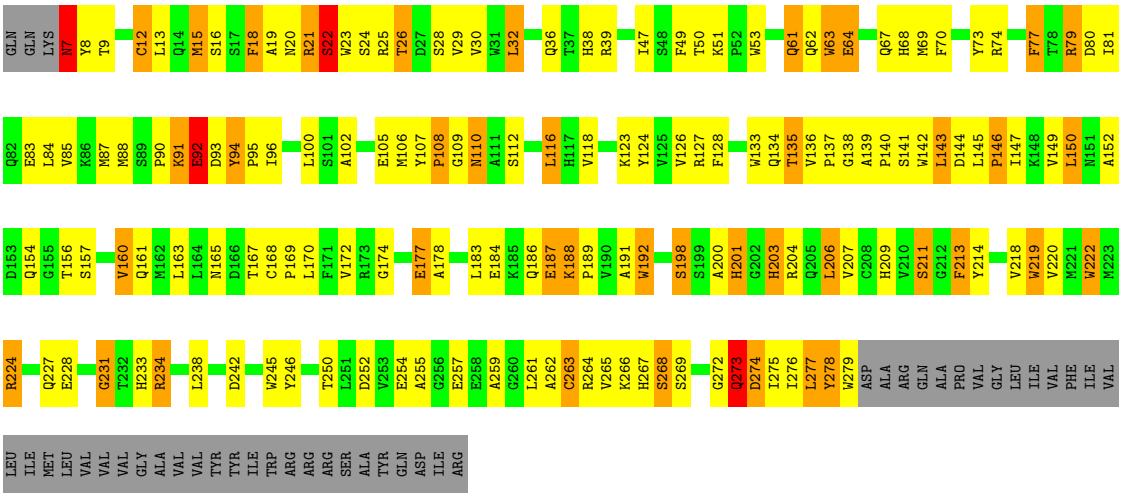
• Molecule 1: CD1

Chain A: 37% 38% 10% • 13%



• Molecule 1: CD1

Chain C: 36% 36% 13% • 13%



• Molecule 2: CD1

Chain B: 46% 41% 10% •

I1 Q2 K3 T4 P5 Q6 I7 Q8 V9 Y10 S11 R12 H13 P14 N21 I22 L23 N24 C25 Y26 V27 T28 Q29 F30 H31 P32 I35 E36 M39 K44 P47 K48 V49 E50 M51 M54 S55 F56 S57 K58 D59 W60 S61 F62 Y63 A66 H67 T68 E69 F70 T73 E74

T75 V82 K83 H84 E89 P90 W95 D96 R97 D98 N99

- Molecule 2: CD1

Chain D: 46% 40% 13%

I1 Q2 K3 T4 P5 Q6 I7 Q8 V9 Y10 S11 R12 H13 P14 P15 E16 N17 G18 K19 I22 L23 N24 C25 Y26 V27 T28 Q29 F30 P33 H34 I35 E36 M39 L40 K41 N42 G43 K44 V49 M54 S55 F56 S57 F62 Y63 I64 L65 T68 E69 F70 T71 P72 T73

E74 T75 D76 T77 Y78 R81 V82 K83 H84 D85 S86 M87 A88 E89 P90 V93 Y94 W95 D96 R97 D98 M99

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	59.34Å 76.20Å 103.40Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	10.00 – 2.67	Depositor
% Data completeness (in resolution range)	83.7 (10.00-2.67)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6026	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.77	18/2257 (0.8%)	1.63	27/3069 (0.9%)
1	C	1.78	21/2257 (0.9%)	1.51	15/3069 (0.5%)
2	B	1.76	6/847 (0.7%)	1.52	5/1148 (0.4%)
2	D	1.76	5/847 (0.6%)	1.52	8/1148 (0.7%)
All	All	1.77	50/6208 (0.8%)	1.56	55/8434 (0.7%)

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ARG	CZ-NH1	7.53	1.42	1.33
1	A	264	ARG	CZ-NH2	7.46	1.42	1.33
1	C	278	TYR	CD2-CE2	6.81	1.49	1.39
1	C	22	SER	CA-CB	6.59	1.62	1.52
1	A	124	TYR	CD1-CE1	6.42	1.49	1.39

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ARG	NE-CZ-NH2	-10.43	115.09	120.30
2	D	81	ARG	NE-CZ-NH2	-8.45	116.08	120.30
2	D	30	PHE	CB-CG-CD1	8.18	126.53	120.80
1	A	74	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	C	204	ARG	NE-CZ-NH1	-7.41	116.60	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2192	0	2097	120	0
1	C	2192	0	2097	136	0
2	B	821	0	796	41	0
2	D	821	0	796	37	0
All	All	6026	0	5786	325	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 28.

The worst 5 of 325 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:C:198:SER:HB2	1:C:201:HIS:HE1	1.26	1.00
1:C:102:ALA:HB2	1:C:116:LEU:HD23	1.43	0.97
1:C:9:THR:HG23	1:C:105:GLU:HG2	1.47	0.96
1:C:88:MET:HG3	1:C:92:GLU:HA	1.47	0.93
1:C:168:CYS:HB3	1:C:169:PRO:HD3	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	271/315 (86%)	229 (84%)	33 (12%)	9 (3%)	4 7
1	C	271/315 (86%)	232 (86%)	33 (12%)	6 (2%)	6 15
2	B	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	4 8
2	D	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	7 16
All	All	736/828 (89%)	635 (86%)	81 (11%)	20 (3%)	5 11

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	199	SER
2	B	97	ARG
2	D	29	GLN
1	A	91	LYS

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	238/274 (87%)	203 (85%)	35 (15%)	3 7
1	C	238/274 (87%)	201 (84%)	37 (16%)	2 6
2	B	94/94 (100%)	87 (93%)	7 (7%)	13 29
2	D	94/94 (100%)	83 (88%)	11 (12%)	5 11
All	All	664/736 (90%)	574 (86%)	90 (14%)	3 8

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	92	GLU
1	C	252	ASP
1	C	135	THR
1	C	188	LYS
1	C	273	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	201	HIS
2	D	6	GLN
2	D	84	HIS
2	D	38	GLN
1	C	7	ASN

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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.