



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID : 1GG3
Title : CRYSTAL STRUCTURE OF THE PROTEIN 4.1R MEMBRANE BINDING
DOMAIN
Authors : Han, B.G.
Deposited on : 2000-07-11
Resolution : 2.80 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
<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

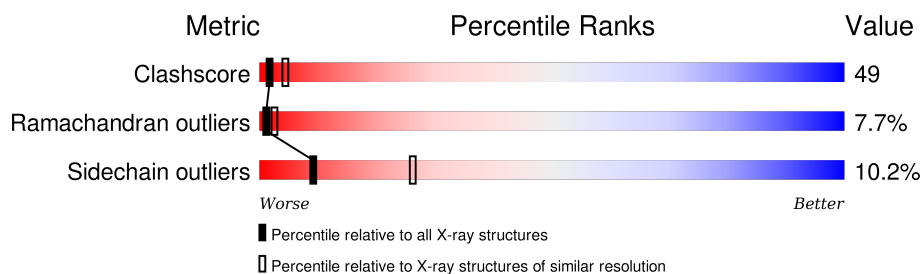
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 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	279	 41% 44% 14%
1	B	279	 43% 48% 9% •
1	C	279	 33% 53% 13% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6837 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 ERYTHROID MEMBRANE PROTEIN 4.1R.

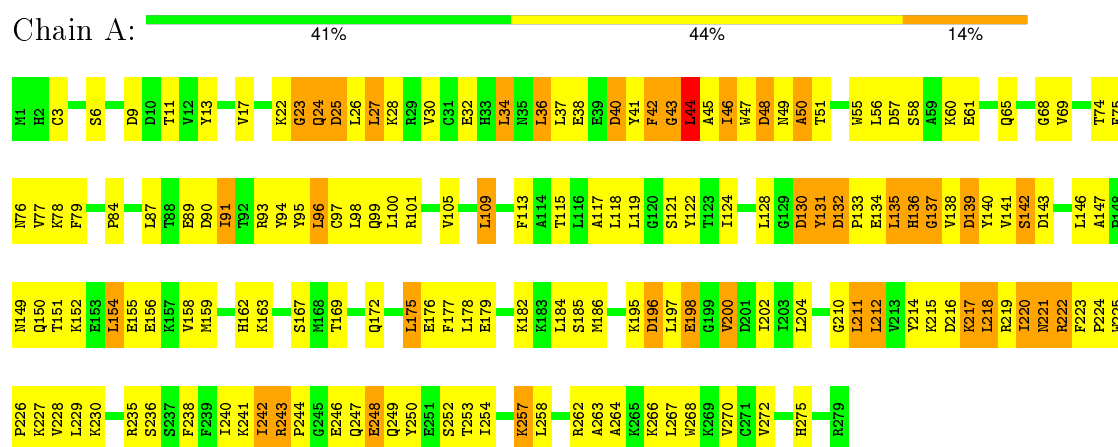
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2279	1472	380	416	11			
1	B	279	Total	C	N	O	S	0	0	0
			2279	1472	380	416	11			
1	C	279	Total	C	N	O	S	0	0	0
			2279	1472	380	416	11			

3 Residue-property plots

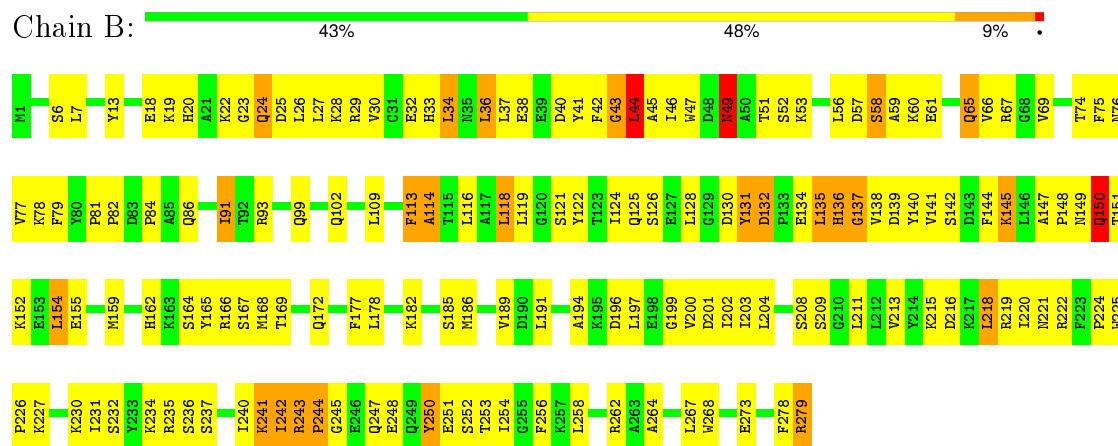
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

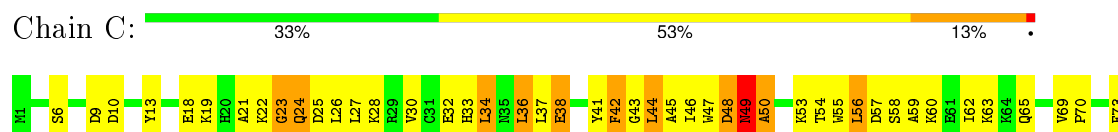
• Molecule 1: ERYTHROID MEMBRANE PROTEIN 4.1R



• Molecule 1: ERYTHROID MEMBRANE PROTEIN 4.1R



• Molecule 1: ERYTHROID MEMBRANE PROTEIN 4.1R



F277	T74	K145	G129
F278	F75	L146	D130
F279	M76	A147	Y131
	V77		D132
	K78	Q150	P133
	F79	T151	E134
	Y80	K152	L136
		E153	H136
		L154	G137
	P84	E155	V138
		L87	D139
		T88	Y140
		E89	V141
		D90	S142
		T91	F144
		T92	
		R93	
		Y94	
		Y95	
		L96	
		C97	
		L98	
		M168	
		Q99	
		L100	
		R101	
		Q102	
		Q172	
		A173	
		D174	
		L175	
		E176	
		F177	
		L178	
		E179	
		K182	
		K183	
		L184	
		S185	
		M186	
		Y187	
		G188	
		V189	
		H192	
		K195	
		D196	
		L197	
		E198	
		G199	
		V200	
		D201	
		I202	
		G205	
		V206	
		C207	
		S208	
		S209	
		G210	
		L211	
		L212	
		V213	
		Y214	
		K215	
		D216	
		K217	
		L218	
		R219	
		T220	
		N221	
		R222	
		F223	
		P224	
		W225	
		P226	
		K227	
		V228	
		L229	
		K230	
		I231	
		K234	
		R235	
		S236	
		S237	
		F238	
		F239	
		T240	
		K241	
		T242	
		R243	
		P244	
		Q247	
		E248	
		Q249	
		Y250	
		E251	
		S252	
		T253	
		I254	
		G255	
		F256	
		K257	
		L258	
		Y261	
		A264	
		K265	
		K266	
		L267	
		W268	
		K269	
		V270	
		C271	
		V272	
		T276	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.90 Å 106.50 Å 93.50 Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.226 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6837	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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	0.46	0/2335	0.71	1/3154 (0.0%)
1	B	0.47	0/2335	0.73	2/3154 (0.1%)
1	C	0.49	0/2335	0.76	1/3154 (0.0%)
All	All	0.48	0/7005	0.73	4/9462 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	LEU	N-CA-C	-5.77	95.43	111.00
1	B	135	LEU	N-CA-C	-5.59	95.92	111.00
1	A	135	LEU	N-CA-C	-5.30	96.69	111.00
1	B	134	GLU	N-CA-C	-5.30	96.69	111.00

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	2279	0	2287	235	0
1	B	2279	0	2287	196	1
1	C	2279	0	2287	251	1
All	All	6837	0	6861	667	2

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 49.

The worst 5 of 667 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:43:GLY:HA2	1:B:79:PHE:H	1.06	1.15
1:A:43:GLY:HA2	1:A:79:PHE:H	1.02	1.12
1:A:229:LEU:HG	1:A:242:ILE:HG12	1.31	1.10
1:C:196:ASP:HB3	1:C:200:VAL:HB	1.32	1.07
1:A:24:GLN:HB2	1:A:28:LYS:HB2	1.35	1.06

All (2) 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:B:251:GLU:OE1	1:B:251:GLU:OE1[2_656]	1.67	0.53
1:C:197:LEU:CD1	1:C:197:LEU:CD1[2_556]	1.68	0.52

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	277/279 (99%)	217 (78%)	36 (13%)	24 (9%)	1	2
1	B	277/279 (99%)	235 (85%)	27 (10%)	15 (5%)	2	7
1	C	277/279 (99%)	209 (76%)	43 (16%)	25 (9%)	1	2
All	All	831/837 (99%)	661 (80%)	106 (13%)	64 (8%)	1	2

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ALA
1	A	136	HIS
1	A	198	GLU

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Mol	Chain	Res	Type
1	A	220	ILE
1	A	242	ILE

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	251/251 (100%)	228 (91%)	23 (9%)	11	32
1	B	251/251 (100%)	222 (88%)	29 (12%)	7	20
1	C	251/251 (100%)	226 (90%)	25 (10%)	9	27
All	All	753/753 (100%)	676 (90%)	77 (10%)	9	26

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
1	B	164	SER
1	C	195	LYS
1	B	109	LEU
1	B	126	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	HIS
1	B	65	GLN
1	C	172	GLN
1	B	33	HIS
1	B	49	ASN

5.3.3 RNA ⓘ

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](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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